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June 2021

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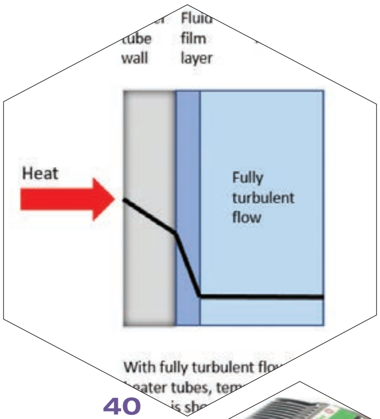

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Coming in July

Look for: **Feature Reports** on Explosion and Overpressure Protection; and Cost Engineering; A **Focus** on Pipes, Tubes and Fittings; A **Facts at your Fingertips** on Adsorbent Materials; a **Newsfront** on Temperature Measurement and Control; **New Products**; and much more

Cover design: Tara Bekman

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Editor's Page

Intelligent machines

By now, we are all used to being surrounded by "smart" machines — smartphones, smart televisions, all sorts of smart appliances at home and smart instruments in our production sites. We are also familiar with connecting our smart devices and sending and receiving information from just about anywhere. And the amount of information that we can gather has increased astronomically, leading to terms like "big data" and to a focus on data analytics in order to put the vast amounts of available information to good use.

Machine learning and artificial intelligence

Alongside this boom in digitalization, more advanced computational techniques and related technologies have given rise to machine learning, where machines do more than just gather and share information, but actually learn through automated data analysis and by identifying patterns. Machines can then predict what will happen and offer recommendations to prevent negative occurrences. One practical application of this is predictive maintenance. When given even broader data resources to process, machines can learn more complex associations, for example facial recognition, in a process termed deep learning.

Machine learning is part of artificial intelligence (AI), which encompasses technologies that allow machines to learn and perform functions that mimic human intelligence. Rapid advances in computer software and storage capabilities, along with the massive increase in data availability through smart devices are enabling broader applications of AI.

Practical AI

Industries are increasingly incorporating AI into their businesses. In a recent survey by McKinsey & Company [*1*], half of the 2,395 participants from a wide range of industries said that their companies have implemented AI in at least one function. The chemical process industries (CPI) are among the adopters of AI. In April, Evonik Industries AG (www.evonik.com) became the world's first chemical company to participate at the MIT-IBM Watson AI Lab (mitibmwatsonailab.mit.edu). The AI Lab is a community of scientists from the Massachusetts Institute of Technology (MIT) and IBM Research who are working with businesses in researching AI. Evonik and IBM had already been investigating AI as partners for several years, and membership in the AI Lab extends this cooperation.

As another example, in December, Covestro AG (www.covestro.com) announced several pilot projects using AI. The company is, for instance, using digital technologies to optimize the manufacturing process for polyesters and to predict peak steam consumption at production plants.

In this issue

There are many practical applications for machine learning and AI being pursued by the CPI. To learn more, see our Newsfront "Artificial Intelligence: Advancing Applications in the CPI" on pp. 12–18.

And our two-part Cover Story on process analytical technology (PAT; pp. 24–34) explores exciting advances in process analyzer technologies. There is also much more in this issue and we hope you enjoy reading. ■

Dorothy Lozowski, Editorial Director

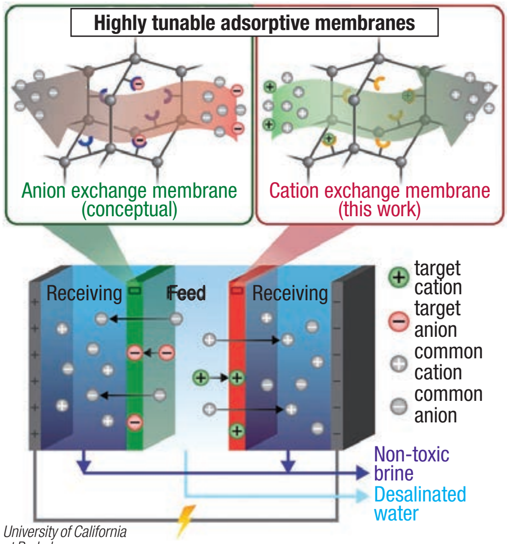
1. McKinsey & Company, The State of AI in 2020, November 17, 2020; www.mckinsey.com/business-functions/mckinsey-analytics/our-insights/global-survey-the-state-of-ai-in-2020

Simultaneous desalination and decontamination of water

The purification of seawater and wastewater for agriculture and human consumption is becoming increasingly important in water-scarce regions. Along with the removal of salt, rendering ocean water and wastewater suitable for humans and plants also involves removal of elements that can be toxic, including mercury, arsenic, lead, uranium, boron and others. While this would usually require several processing steps, a research team led by University of California at Berkeley (www.berkeley.edu) scientists has fabricated a flexible ion-exchange polymer membrane that can selectively adsorb heavy metals at the same time that it removes salt, in a process they call "ion-capture electrodialysis."

The new technique is designed to be easily added to current membrane-based electrodialysis desalination processes (where electric voltage drives salt ions through the membrane), as well as diffusion dialysis systems. The Berkeley team incorporated porous aromatic framework (PAF) nanoparticles into sulfonated polymer membranes to capture metals contaminating the water.

PAFs are three-dimensional networks of carbon atoms connected by aromatic linkers. Various molecules can be attached to the aromatic linkers to capture specific chemicals. Salts are removed from the water with a series of cation- and anion-exchange membranes, and the embedded PAF particles are selected to capture specific target ions, removing either a single type of valuable ion (gold or copper, for example), or multiple contaminants at the same time, the research team explains (diagram).



University of California at Berkeley

The Berkeley team says the reusable polymer membrane containing the PAF nanoparticles is stable in water and at elevated temperatures, unlike most metal organic frameworks (MOFs), for example. The researchers hope to be able to tune the nanoparticles to remove other types of toxic chemicals, including PFAS (polyfluoroalkyl substances). The group's work was recently published in the journal *Science*.

A new way to capture CO_2 in cement

Technologies designed to capture and store CO_2 emissions from industrial operations are rapidly gaining traction, but finding ways to economically utilize the captured CO_2 has posed challenges. A team of engineers from the University of California Los Angeles' (UCLA; www.ucla.edu) Institute for Carbon Management have developed a new cement formulation, into which captured CO_2 emissions are directly infused.

Traditional cement is based on calcium silicate, but the new CO_2-infused cement, branded under the name CarbonBuilt, uses hydrated lime, which is known to quickly absorb CO_2. The team developed a new method, wherein as CarbonBuilt concrete hardens and strengthens, captured CO_2 is quickly absorbed and permanently trapped. When compared to traditional concrete, the CarbonBuilt formulation reportedly reduces concrete's carbon footprint by more than 50%, all while demonstrating comparable strength and durability. Contributing to this footprint reduction is CarbonBuilt's Reversa process, which promotes the re-use of waste streams like flyash while significantly reducing the amount of cement binder needed to produce concrete. Furthermore, the process does not require operation at extreme temperature or pressure. Another benefit of capturing CO_2 in cement is that, unlike other CO_2-mitigation methods, gas captured from industrial fluegas can be directly utilized without additional purification or conversion steps.

Last year, the team began an industrial-scale demonstration of its process in Wyoming that produced around 150 metric tons of CarbonBuilt concrete. A second demonstration was recently completed at the National Carbon Capture Center in Alabama, producing more than 5,000 concrete blocks using CO_2 emissions from coal and natural-gas power plants. Each block can store around 0.75 lb of CO_2. The team expects to significantly scale up production capacities in the coming years.

Edited by:
Gerald Ondrey

BIOMASS

Corn stover is among the major feedstocks for biorefineries, and can be converted to bioethanol. When corn stover contains moisture above certain levels, it can clog conveyers and chutes during processing, leading to operational problems and process stoppages. To eliminate moisture-related stoppages at biorefineries, scientists at Los Alamos National Laboratory (Los Alamos, N.M.; www.lanl.gov) collaborated with bulk-solids-handling engineers at Jenike & Johanson (Tyngsboro, Mass.; www.jenike.com) to develop Smart Transfer Chutes. The biomass-handling chutes are outfitted with acoustic moisture sensors for continuous, realtime monitoring of corn stover moisture levels. The acoustic moisture sensors work by directing soundwaves through the corn stover as it is being processed. If moisture contents exceed those that are known to cause stoppages, it sends a signal to a computer, which engages a track change on the conveyor belt, redirecting it to be further dried. The system improves the operational efficiency of biomass processing and helps improve the cost-effectiveness of biofuels, the researchers say.

CRYSTALLIZATION

Last month, Comprimo — the sulfur technology business of Worley (North Sydney, Australia; www.worley.com) — acquired the rights to license the Eutectic Freeze Crystallization (EFC) technology from Cool Separations B.V. (Poortugaal, the Netherlands; www.

(Continues on p. 6)

coolseparations.nl). When an EFC unit is combined with Comprimo's desulfurization technologies (SuperClaus or EuroClaus with a caustic scrubber), this process eliminates gaseous and liquid sulfur emissions from the scrubber effluent and provides clean reusable water. In addition to treating this highly contaminated effluent to recover water, the process also produces sellable salt, which can be used as a potential raw material for fertilizer industries.

SURFACTANTS

Unilever (London, U.K.; www.unilever.com) has partnered with LanzaTech, Inc. (Skokie, Ill.; www.lanzatech.com) and India Glycols Ltd. (Noida, India; www.indiaglycols.com) to produce a surfactant made from industrial carbon emissions instead of from fossil fuels. The shift in production utilizes biotechnologies and a newly configured supply chain between the three partners, who are working together for the first time.

The three-stage process marks the first time a surfactant made using captured carbon emissions will come to market in a cleaning product. First, LanzaTech uses biotechnology to capture waste industrial emissions at its Beijing Shougang LanzaTech plant in China and converts these emissions to ethanol. India Glycols then converts the ethanol into ethylene oxide, a key feedstock to make surfactants at its site in India. Unilever then uses the surfactant in the new OMO (Persil) laundry capsules, manufactured at its Hefei factory in China. The new laundry capsule was launched in China on April 22nd, World Earth Day.

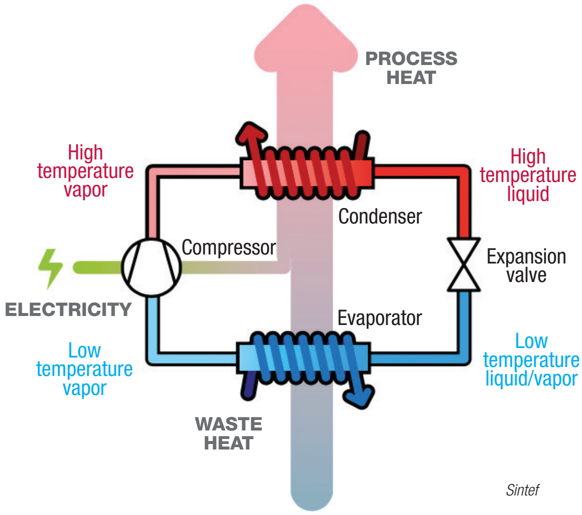
MEMBRANES

A research group from the Graduate School of

(Continues on p. 7)

High-temperature heat pump promises significant energy savings

Industrial heat pumps (diagram) are a relatively mature technology that converts low-temperature waste heat into a more usable heat at a higher temperature (above the "pinch point"). However, the technology has been limited to applications of up to 100°C. Now, a new heat pump that can produce process heat at temperatures up to 180°C has been developed in Norwegian project, called Free2Heat — a spinoff generated at the HighEFF Center for Environmentally Friendly Energy Research at Sintef (Trondheim; www.sintef.no). The higher temperature will make the application of heat pumps more useful for producing process heat for the chemical process industries (CPI), as opposed to space heating applications that are commonly used in houses and buildings.



Sintef

Developed by project partners Sintef, the Norwegian University of Science and Technology (NTNU; Trondheim; www.ntnu.edu) and compressor-manufacturer ToCircle Industries A/S (Oslo; www.tocircle.com), the new heat pump is a concept demonstration of a technology initially developed by the first two partners for processing a dairy product line at TINE (Bergen, Norway). That system, described in a recent issue of *Applied Thermal Engineering*, used a hybrid absorption-compression heat pump (HACHP) with natural refrigerants to produce process heat at 100°C, which enabled the company to reduce its total energy consumption by up to 50% and become the world's first zero-emissions dairy.

For the new high-temperature heat pump, water is used as the refrigerant and a rotary vane device, developed by ToCircle, is used as the compressor. The ToCircle compressor uses water as the lubricant, which avoids problems associated with lubricants in the steam system, says Sintef researcher Michael Bantle.

The project, launched in 2019, will continue to 2024. By the end of this year, ToCircle plans to have a 500 kW_{th} compressor commercially available, which can be used for steam-producing heat pumps.

Modular waste-to-energy system is cost-competitive at smaller scales

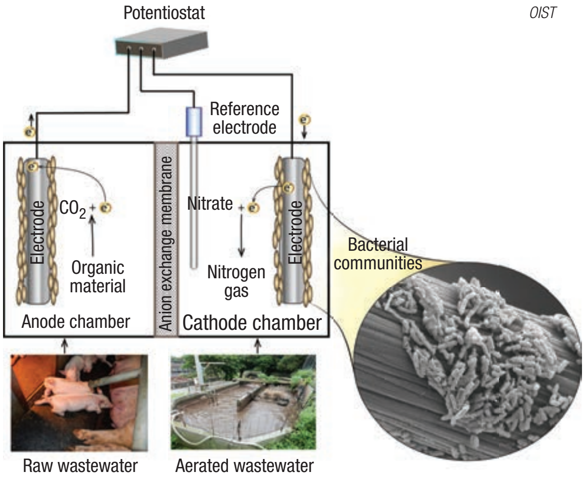
A newly launched modular waste-to-energy system is capable of delivering off-grid heat and power with competitive economics to a variety of locations, including military bases, remote sites and commercial installations, according to creator Enexor BioEnergy LLC (Franklin, Tenn.; www.enexor.com). Under a contract from the U.S. Army Corps of Engineers announced in April, the company is testing the proprietary units, known as Bio-CHP, on locally generated organic waste from U.S. Navy vessels and bases.

The Bio-CHP units are housed in 20-ft custom shipping containers that can be trucked to various locations to provide combined heat and power by combusting organic material, such as food waste, agricultural waste, seaweed, wood waste and others. Enexor has also designed a companion unit to combust common, non-chlorinated packaging plastics, such as polyethylene (PE), polypropylene (PP) and polyethylene terephthalate (PET).

"These 'behind-the-meter' energy units are based on advanced combustion, not on gasification, which tends not work economically at smaller scales," explains Enexor CEO Lee Jestings. "Among the keys to the technology is a specially designed turbine that was custom-made for this application, as well as a high-temperature ceramic filter for cleaning the exhaust stream, and advanced heat exchangers."

Rather than selling the modular units, Enexor is using an "energy-as-a-service" model, where the user will pay for the heat and power consumed onsite, but the company will own the units. "Application areas for these units include any location where organic waste is generated, such as food-processing facilities, military installations, distilleries, island resorts and others," Jestings says.

An electrotrophic system that treats swine sewage in one step



OIST

Researchers from the Biological Systems Unit at the Okinawa Institute of Science and Technology Graduate University (OIST; Japan; www.oist.jp) have developed a bioelectrochemical system that uses bacterial communities to break down organic material from raw wastewater, and removes both nitrates and phosphates from aerated wastewater. A proof-of-concept have been demonstrated in both the laboratory and on a local swine farm in Okinawa, Japan.

Across Okinawa, large amounts of wastewater are produced by pig farms. The traditional aeration system currently utilized by farmers mainly treats organic matter in the wastewater and also converts the ammonium present to nitrate, but it does not treat the nitrate further. In Japan, the nitrate discharge limit for the livestock industry will soon be lowered to one fifth of the current 500-mg/L level — more than 35% of farms in Okinawa are likely to exceed this impending change, according to OIST.

"Our new system uses two different chambers," explains Anna Prokhorova, lead author of an article recently published in *Bioresource Technology*. "In one chamber, full strength swine wastewater is treated for the removal of odor, pathogens and organic matter, whereas in the other chamber, excess nitrate and phosphate is removed from wastewater that has already been treated through the traditional aeration system. To the best of our knowledge, this is the first system to successfully treat two different types of wastewater at the same time," she says.

In the anode chamber, bacteria react with the organic molecules present, releasing electrons in the process (diagram). These electrons are then transferred to the cathode chamber via the electrodes. The cathode chamber contains wastewater that has already gone through the aeration process and thus has high levels of nitrate. Bacteria on the surface of the cathode chamber accept these electrons and use them to power the conversion of nitrates to nitrogen gas.

Engineering at Tohoku University (Japan; www.tohoku.ac.jp) has developed an ion-selective, smart porous membrane that can respond to external stimuli for controlling permeation. The technology has potential applications in molecular separation and sensing applications.

Nanostructure properties, such as pore size, thickness and film density, affect molecular selectivity and molecular permeability. Surface properties also have a significant impact on molecular selectivity. Therefore, it is important to be able to control both the 3-D nanostructures and surface properties of ultrathin porous films.

"In our study, we succeeded in developing responsive porous SiO_2 thin films with an extremely thin film thickness of 8 nm with a uniformly covered surface in a pH-responsive silane coupling agent," says Yuya Ishizaki, a co-author of the study published in *Langmuir*. "The responsive porous thin film can adjust the surface charge depending on the pH change in the solution, resulting in selective ion permeation."

To prepare the porous films with a controlled structure to nanometer-scale accuracy, the research group focused on

(Continues on p. 8)

Reducing the cost of redox flow batteries

Redox flow batteries (RFBs) are a promising alternative to lithium-ion batteries for storing large quantities of renewable energy (see *Chem. Eng.*, September 2016, pp. 14–20), but they have always been too expensive for the mass market. Now, researchers at the Fraunhofer Institute for Environmental, Safety and Energy Technology (Umsicht; Oberhausen, Germany; www.umsicht.fraunhofer.de) have completely redesigned the heart of a RFB — the stack — resulting in a "massive" reduction in material usage and costs.

"The stack that has been developed is 40% more cost-effective in terms of material costs," says professor Christian Doetsch. "Production costs have also been significantly reduced. The stack weighs 80% less than a conventional stack and is only about half the size," he adds.

Stacks usually comprise 160 stacked components that are held together by a large number of screws and solid metal plates and sealed with numerous gaskets. Some of these components are injection molded, meaning they are brittle. To avoid this problem, the team of researchers used similar base materials — graphite and carbon black — but approached the process differently: plastic pellets are cooled to temperatures as low as –80°C, then ground into powder and mixed with 80 wt.% graphite. The powder is sent through a system of several rollers moving at different speeds and heated to different temperatures. As a result, the powder is briefly melted between the rollers at moderate temperatures and low pressures, and then kneaded and rolled up. The process makes it possible to manufacture bipolar plates of up to several square meters in size. This powder-to-roll process is the key to reducing production costs, because very thin (0.1–0.4 mm) plates can be produced. Because less material is used, the costs, weight and footprint of the device are reduced.

The stack is being marketed by the spin-off Volterion GmbH (Dortmund, Germany; www.volterion.de). The company has already built and sold more than a thousand stacks. Christian Doetsch and Lukas Kopietz from Fraunhofer Umsicht and Thorsten Seipp from Volterion have been awarded the Joseph von Fraunhofer Prize for this development.

polymer thin films containing silsesquioxanes, which have unique cage structures. The polymer films were fabricated using the Langmuir-Blodgett technique, chosen because it provides molecular-scale controllability in the film thickness. Langmuir-Blodgett polymer nanosheets also make it possible to fabricate porous SiO_2 thin films with controlled nanostructures by simple ultraviolet (UV) light irradiation under ambient conditions.

5-HMF

Sulzer Chemtech Ltd. (Winterthur, Switzerland; www.sulzer.com) and AVA Biochem AG (Zug, both Switzerland; www.ava-biochem.com) have entered into an exclusive license agreement to commercialize AVA Biochem's COBRIS technology (Conversion of Biomass to Renewable Industrial Substances). COBRIS offers a versatile solution to produce 5-(hydroxymethyl) furfural (5-HMF), a bio-based platform chemical that is a building block for the production of a broad range of widely used chemical products.

AVA Biochem's proprietary water-based COBRIS hydro-thermal process (HTP) converts sugar-rich biomass into 5-HMF, a renewable and non-toxic compound that can be used to produce commodity chemicals, such as adhesives, food additives, textile fibers, packaging, films and fine chemicals, as well as a possible alternative to formaldehyde used in chipboards.

Sulzer Chemtech will commercialize the licensed technology, along with its proprietary key equipment for the purification of 5-HMF, such as falling-film evaporators. These are already supporting operations at the unique demonstration plant in Muttenz, Switzerland, where 5-HMF is produced in different forms, for a total capacity of 6 m.t./yr.

HEX RECYCLING

Alfa Laval AB (Lund; www.alfalaval.com), in partnership with Stena Recycling AB (Göteborg, both Sweden; www.stenarecycling.com), plan to launch a new business model for sustainable and environmentally efficient recycling of heat exchangers (HEXs), enabling up to 100% metal regeneration. The partnership is a first step towards a circular approach to the company's product portfolio, and an important part of Alfa Laval's commitment to become carbon neutral by 2030. ❐

Converting woody biomass to intermediates allows carbon-negative products

Construction has begun on a market demonstration facility for manufacturing chloromethyl furfural (CMF) and hydrothermal carbon (HTC) from a variety of waste biomass feedstocks. With subsequent chemical transformation, these flexible intermediates can be converted into final products, such as polyethylene terephthalate (PET) packaging and carbon black, that are carbon-negative (net removal of CO_2 from the atmosphere), according to an ISO-compliant third-party lifecycle analysis (LCA).

The new market demonstration facility, being built by Origin Materials (West Sacramento, Calif.; www.originmaterials.com) in Sarnia, Ont., will eventually consume 25,000 tons per year of feedstock. It is expected to be completed at the end of 2022. Origin is also planning a world-scale commercial facility to be completed in 2025.

"Many companies have made 'net-zero' carbon commitments without fully appreciating the carbon footprint of the materials from which their products are made," explains John Bissell, co-founder and CEO of Origin Materials. "This unique platform technology allows a pathway for a range of carbon-negative final products."

The process works by feeding woodchips or other biomass, such as pulp waste, rice hulls, or cardboard, into a reactor containing hydrochloric acid (HCl), organic solvents and catalyst material. The reactor converts C6 sugars bound in cellulose into CMF, and C5 sugars from hemicellulose into furfural and levulinic acid. The lignin in the biomass is converted to HTC. The process is a reactive extraction, after which an aqueous phase containing the HTC is separated from the organic phase. The organic phase is sent to distillation, which yields the major product (CMF) and recovers the solvent.

"Once the CMF is converted to *para*-xylene, it can link up to the existing supply-chain infrastructure for PET bottles and packages," Bissell notes, and "carbon black can be made from the HTC with two desirable qualities: particle morphologies that are similar to those of petroleum-derived carbon black and no detectable polyaromatic hydrocarbons (PAHs), which are human carcinogens."

Bissell says the company has established offtake agreements for products made from the chemicals produced at the new facility.

Improve aircraft fuel efficiency with 'sharkskin'

Lufthansa Technik AG (Hamburg; www.lufthansa-technik.com) and BASF SE (Ludwigshafen, Germany; www.basf.com) have developed a surface film, tradenamed AeroSHARK, that mimics the fine structure of a shark's skin for reducing friction. The technology is to be rolled out on Lufthansa Cargo AG's (Frankfurt am Main, Germany; www.lufthansa-cargo.com) entire freighter fleet from the beginning of 2022, making the aircraft more economical and reducing emissions.

The surface structure, consisting of riblets — tiny (around 50 µm) grooves arranged longitudinally along the flow — that imitates the properties of sharkskin and therefore optimizes the aerodynamics on flow-related parts of the aircraft. This means that less fuel is needed overall. For Lufthansa Cargo's Boeing 777F freighters, Lufthansa Technik estimates a drag reduction of more than 1%. For the entire fleet of ten aircraft, this translates to annual savings of around 3,700 tons of kerosene and just under 11,700 tons of CO_2 emissions — the equivalent of 48 individual freight flights from Frankfurt to Shanghai.

The riblet surface is an example of functional films being developed by the Coatings division of BASF (www.basf-coatings.com) in its Beyond Paint Solutions unit. A solution was implemented together with Lufthansa Technik that fulfills the strict requirements of the aviation industry. Exterior surfaces used in aviation are exposed to factors, such as strong ultraviolet (UV) radiation, as well as temperature and pressure fluctuations at high altitudes, among others. BASF has therefore focused its development on achieving extreme durability and weather resistance. The key criteria for use in aviation operation include simple application and handling as well as ease-of-repair, for which a custom concept has been developed.

Lufthansa Technik and BASF plan to continue developing the new technology consistently to include additional aircraft types and even larger surfaces so that they can support airlines around the globe even more comprehensively in the future in reaching their sustainability goals. Initial model calculations show that use of sharkskin technology at its highest expansion level could reduce CO_2 emissions by as much as 3%. ■

Business News

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Plant Watch

BASF to expand PGM recycling capacity in South Carolina

May 12, 2021 — BASF SE (Ludwigshafen, Germany; www.basf.com) is expanding its platinum group metals (PGM) refining facility in Seneca, S.C. New capital investments will increase refining capacity to recycle precious metals from spent catalysts, such as automotive catalytic converters.

Mitsui Chemicals starts production of hydrocarbon-based synthetic fluids

May 12, 2021 — Mitsui Chemicals, Inc. (Tokyo, Japan; www.mitsuichemicals.com) started commercial production at a new plant to produce hydrocarbon-based synthetic fluids in Ichihara, Chiba, Japan. According to Mitsui Chemicals, this plant is producing the world's first hydrocarbon-based synthetic-fluid product to be offered commercially. The product is expected to find use as a viscosity modifier for gear oils, as well as industrial lubricants and greases.

Trinseo announces commercial-scale production of recycled PS via dissolution

May 10, 2021 — Trinseo (Berwyn, Pa.; www.trinseo.com) recently commercialized its production method for recycled polystyrene (PS) from dissolution and is offering a new material using this process. With this recycling method, post-consumer recycled (PCR) material is dissolved in a solvent followed by a series of purification steps to separate the polymer from additives and contaminants. The material is fed into a polymerization reactor train, resulting in a PS polymer with 30% PCR content.

Chevron Phillips to build world-scale 1-hexene plant in Old Ocean, Texas

May 6, 2021 — Chevron Phillips Chemical L.P. (The Woodlands, Tex.; www.cpchem.com) plans to build a second world-scale unit to produce on-purpose 1-hexene. Expected capacity for the new unit is 266,000 metric tons per year (m.t./yr), with targeted startup in 2023. Its location will be Old Ocean, Tex., near the company's Sweeny facility.

LyondellBasell produces first polymers using plastic-waste feedstock

May 6, 2021 — LyondellBasell Industries N.V. (Rotterdam, the Netherlands; www.lyondellbasell.com) has produced new polymers using raw materials derived from plastic waste at its Wesseling, Germany site. Produced by the thermal conversion of plastic waste, this raw material is converted into ethylene and propylene, and then processed into polypropylene (PP) and polyethylene (PE) in downstream units.

Hanwha Total Petrochemical commissions new polypropylene unit

May 6, 2021 — Total SE (Paris, France; www.total.com) announced that its Hanwha Total Petrochemical (HTC) joint venture is commissioning a new PP line at the Daesan integrated refining and petrochemical complex in South Korea, adding a further 60% to its production capacity, which now totals 1.1 million m.t./yr. The site will also increase its ethylene production capacity by 10% to 1.5 million m.t./yr.

Neste to increase SAF production capacity at Rotterdam refinery

May 4, 2021 — Neste Corp. (Espoo, Finland; www.neste.com) will modify its Rotterdam refinery to enable production of sustainable aviation fuel (SAF). Currently, the plant produces mainly renewable diesel. The modifications to the refinery, involving an investment of approximately €190 million, will give Neste the option to produce up to 500,000 m.t./yr of SAF as part of the site's existing capacity. Neste expects the project to be completed in the second half of 2023.

Phillips 66 completes hydrotreater conversion for renewable fuel production

May 3, 2021 — Phillips 66 (Houston; www.phillips66.com) completed a diesel hydrotreater conversion project at its San Francisco Refinery in Rodeo, Calif., which will ramp up to 8,000 barrels per day (bbl/d) of renewable diesel production by the third quarter of 2021. Subject to permitting and approvals, full conversion of the refinery is expected in early 2024. Upon completion, the facility will have over 50,000 bbl/d (800 million gal/yr) of renewable-fuel production capacity.

Nouryon and Atul start up monochloroacetic acid plant in India

April 27, 2021 — Nouryon (Amsterdam, the Netherlands; www.nouryon.com) and Atul successfully started production at their Anaven joint venture project in Gujarat, India. Anaven is India's largest monochloroacetic acid (MCA) production site, with a current MCA production capacity of 32,000 m.t./yr. This includes the potential for a rapid expansion of up to 60,000 m.t./yr.

Mergers & Acquisitions

Nouryon to separate its base-chemicals business into standalone company

May 12, 2021 — Nouryon announced its intention to spin-out its base-chemicals business, Nobian, into a separate company that will produce essential base chemicals for a wide range of industry sectors, including

construction, cleaning, pharmaceuticals and water treatment. Nobian employs about 1,600 people and had revenues of €1.0 billion in 2020. The separation is expected to be completed by the third quarter of 2021.

Altana acquires of Henkel's closure-materials business

May 10, 2021 — Altana AG (Wesel, Germany; www.altana.com) has acquired the closure materials business of Henkel AG & Co. KGaA (Düsseldorf, Germany; www.henkel.com), strengthening its range of PVC-free solutions for the packaging industry. The acquired business will be integrated into Altana's Actega division and globally assigned to the metal packaging solutions business line.

Shell sells Puget Sound Refinery to HollyFrontier for $350 million

May 5, 2021 — HollyFrontier Corp. (Dallas, Tex.; www.hollyfrontier.com) has entered into a definitive agreement to acquire the 149,000-bbl/d Puget Sound Refinery, as well as an onsite cogeneration facility and related logistics assets, from Equilon Enterprises LLC, a subsidiary of Royal Dutch Shell N.V. (Rotterdam, the Netherlands; www.shell.com). The purchase price is $350 million, plus hydrocarbon inventory to be valued at closing with an estimated value in the range of $150 to $180 million.

BASF and Umicore enter into a patent cross-license agreement

May 4, 2021 — BASF and Umicore N.V. (Brussels, Belgium; www.umicore.com) have entered into a non-exclusive patent cross-license agreement covering a broad range of cathode active materials and their precursors, including chemistries such as nickel cobalt manganese (NCM), nickel cobalt aluminum (NCA), nickel cobalt manganese aluminum (NCMA) and lithium-rich, high-manganese high-energy NCM (HE NCM). The agreement covers more than 100 patent families filed in Europe, the U.S., China, Korea and Japan.

Eastman acquires nutrition-additives manufacturer in Spain

April 30, 2021 — Eastman Chemical Co. (Kingsport, Tenn.; www.eastman.com) has acquired 3F Feed & Food, a Spain-based specialist in the technical and commercial development of feed additives. 3F's business and assets will become part of Eastman's Additives & Functional Products segment. Included in the acquisition is 3F's product portfolio of food and feed additives, a state-of-the-art production facility located in Avila, Spain, in-house application and development capabilities and technical service capabilities.

Sika to acquire adhesives business from Yokohama Rubber

April 28, 2021 — Sika AG (Baar, Switzerland; www.sika.com) plans to acquire Hamatite, the adhesives business of The Yokohama Rubber Co. (Tokyo, Japan; www.y-yokohama.com). Hamatite operates five manufacturing plants, supplying adhesives and sealants to the automotive and construction industries. The main plant is in Hiratsuka, Japan, and additional manufacturing facilities are located in Japan, China, Thailand and the U.S. Hamatite has generated annual sales of around CHF 160 million ($175 million). ■

Mary Page Bailey

Artificial Intelligence: Advancing Applications in the CPI

A convergence of digital technologies and data science means that industrial AI is gaining ground and producing results for CPI users

As data accessibility and analysis capabilities have rapidly advanced in recent years, new digital platforms driven by artificial intelligence (AI) and machine learning (ML) are increasingly finding practical applications in industry.

"Data are so readily available now. Several years ago, we didn't have the manipulation capability, the broad platform or cloud capacity to really work with large volumes of data. We've got that now, so that has been huge in making AI more practical," says Paige Morse, industry marketing director for chemicals at Aspen Technology, Inc. (Bedford, Mass.; www.aspentech.com). While AI and ML have been part of the digitalization discussion for many years, these technologies have not seen a great deal of practical application in the chemical process industries (CPI) until relatively recently, says Don Mack, global alliance manager at Siemens Industry, Inc. (Alpharetta, Ga.; www.industry.usa.siemens.com). "In order for AI to work correctly, it needs data. Control systems and historians in chemical plants have a lot of data available, but in many cases, those data have just been sitting dormant, not really being put to good use. However, new digitalization tools enable us to address some use cases for AI that until recently just weren't possible."

This convergence of technologies, from smart sensors to high-performance computing and cloud storage, along with advances in data science, deep learning and access to free and open-source software, have enabled the field of industrial AI to move beyond pure research to practical applications with business benefits, says Samvith Rao, chemical and petroleum industry manager at MathWorks (Natick, Mass.; www.mathworks.com). Such business benefits are wide-ranging, spanning varying realms from maintenance to materials science to emerging applications like supply-chain logistics and augmented-reality (AR). MathWorks recently collaborated with a Shell petroleum refinery to use AI to automatically incorporate tagged equipment information into operators' AR headsets.

Another major emerging area for industrial AI is in supply-chain management. "The application of AI in supply chains lets us look at different scenarios and consider alternatives. Feedback from data about what's actually occurred, including any surprising events, can be put into the model to develop better scenario options that appropriately reflect reality," says Morse.

Implementing AI practically

With the wide variety of end-use applications and ever-expanding platform capabilities, determining the most streamlined way to adopt an AI-based platform into an existing process can seem daunting, but Colin Parris, senior vice president and chief technology officer at GE Digital (San Ramon, Calif.; www.ge.com/digital), classifies industrial AI into three discrete pillars that build upon each other to deliver value — early warning of problems, continuous prediction of problems and dynamic optimization. Data are, of course, paramount in realizing all three pillars. "For early warning, I have sensors to give the state of the plant, showing the anomalies when that state changes. Continuous prediction looks at condition-based data to avoid unplanned shutdowns. Here, I want to know the condition of the ball bearings, the corrosion in the pipes, understand the creep in the machines in order to then determine the best plan and not default to time-based maintenance, so I need a lot of data. And if I want to do optimization, I need even more data," says Parris. All of the data can be culminated into a digital twin, which Parris defines as a "living, learning" model that is continuously updated to give an exact view of an asset (Figure 1).

FIGURE 1. A robust digital twin may look at an entire plant, or might be a slimmed-down model that considers only certain critical parts. The model should use AI to continuously update itself

GE Digital worked with Wacker Chemie AG (Munich, Germany; www.wacker.com) to apply a holistic AI hierarchy for asset-performance management (APM) at a polysilicon production plant in Tennessee. There are roughly 1,500 pressure vessels at the site, and maintenance on them takes six weeks, resulting in significant financial burden due to lost production time. "Regulatory compliance meant that these vessels were supposed to be maintained every two years. But, because we were able to actually capture the digital twin and show the current state of the asset, we helped the plant achieve API 580/581 certification, which says if a plant can show a certain level of condition-based capability, they can extend the mainte-

nance interval anywhere from 5 to 10 years based upon the condition," explains Parris. With the early-warning and continuous-prediction pieces in place, the plant was experiencing improved availability and less downtime, and was able to begin looking at dynamic optimization. For Wacker, this included investigating specific product characteristics and intelligently adjusting the processes for higher-margin products. "That's the way it tends to work — you go in a stepwise fashion to ultimately get to optimization, but it's really hard to get to the optimization piece unless you first really understand the asset and have a digital twin that you know is learning as you make changes," adds Parris.

Furthermore, when implementing an advanced AI solution in a new or existing process, users must consider how the platform will be used and who will actually be using it. In the past, "black-box" AI solutions required users with some expertise in data science or advanced statistics, which often resulted in organizational data siloes, says Allison Buenemann, industry principal — chemicals, at Seeq Corp. (Seattle, Wash.; www.seeq.com). Now, the industry has more "self-service" offerings in the advanced analytics and ML space, meaning that users in many different roles can access the most relevant data and insights for their own unique job needs. "For instance, frontline process experts can hit the ground running, solving problems using complex algorithms from an unintimidating low- or no-code application experience. Executives and management teams can expect an empowered workforce solving high-value business problems with rapid time to insight," adds Buenemann. This "democratization" of data analytics and ML across organizations means that all stakeholders can work together to drive business value. "Users must be able to document the thought process behind an analysis and they also must be able to structure analysis results for easy consumption," she explains.

Connectivity and collaboration

The massive growth in sensor volume and associated data availability have certainly helped to promote the applicability of AI in industrial environments, but computing power and network connectivity are also critical pieces of the puzzle. Yokogawa Electric Corp. (Tokyo, Japan; www.yokogawa.com) recently announced a proof-of-concept project to utilize fifth-generation (5G) mobile communications for AI-enabled process controllers. The project will focus on using 5G to remotely control the level in a network of water tanks. One of the major benefits of 5G connectivity in autonomous, realtime plant control, according to Hirotsugu Gotou, manager, Yokogawa products control center, is its low-latency function, which means that the network can process a large volume of data with minimal delay. Yokogawa's cloud-based AI controller system employs reinforcement-learning technology to determine the optimal operation parameters for a particular control loop.

FIGURE 2. This demonstration unit includes a three-tank network in which an autonomous, reinforcement-learning-based scheme monitors and controls water level

Understanding reinforcement-learning schemes, which build upon modern predictive control, is crucial for autonomous process control. "Reinforcement learning is a type of machine learning in which a computer learns to perform a task through repeated trial-and-error interactions with a dynamic environment," explains Mathworks' Samvith Rao. Such a platform develops control policy in real time by interacting with the process, enabling the com-

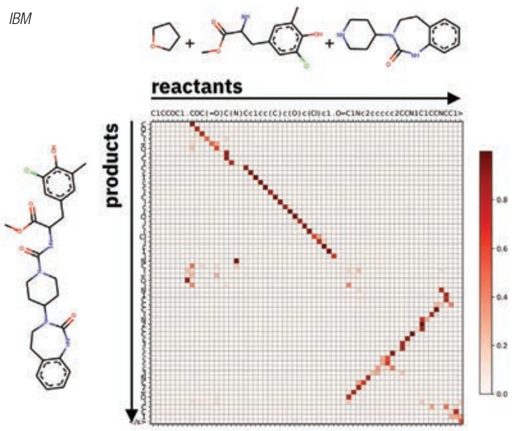


FIGURE 3. AI can be used to quickly determine synthetic routes for new molecules

puter to make a series of decisions that maximize a reward metric for the task without human intervention and without being explicitly programmed to achieve the task. "Robust mechanisms for safe operation of a fully trained model, and indeed, for safe operation of a plant, are high priorities for further investigation," he emphasizes.

In Yokogawa's reinforcement-learning proof-of-concept, the AI controls tank level and continuously receives sensor data on flowrate and level. "Based on these data, the AI will learn about the operation and will repeat the process to derive the optimal operation parameters," explains Gotou. Yokogawa previously completed a demonstration project using its proprietary AI to control water level in a three-tank system (Figure 2), which showed that after 30 iterations of learning (taking less than 4 h), the AI agent was able learn from its past decisions to determine the optimal control methods. Now, the company will work with mobile network provider NTT Domoco to construct a demonstration facility for cloud-based remote control of water tank level and evaluate the communication performance of the 5G network for realtime, autonomous process control. 5G networks are not yet widely adopted in industrial settings, but other projects are also exploring these technologies for IIoT applications. In April, GE Research announced an initiative to test Verizon's 5G platform in a variety of industrial applications, including realtime control of wind farms. And last year, Accenture and AT&T began a 5G proof-of-concept project to develop 5G use cases for IIoT applications at a petroleum refinery in Louisiana operated by Phillips 66.

Another important factor is the collaborative environment that has been fostered through open-source AI platforms, explains Gino Hernandez, head of global digital business for ABB Energy Industries (Zurich, Switzerland; www.abb.com). "As things become more open and more distributed, I think it's going to enable users to apply the technologies in a more meaningful way. The more people talk about the different models and their successes using open-source type AI models, and being able to have platforms where they can import and run those models is going to be key," he notes. In the past, vendors kept their platforms closed, which limited users to develop models only for a specific digital architecture. Now, says Hernandez, more AI platforms enable users to import models — including their own proprietary algorithms — from various sources to develop a more robust analytics program.

As with any digital technology, cybersecurity and protecting proprietary intellectual property (IP) are paramount, but Hernandez also brings up the idea of "sharable IP" as a major area of opportunity for industrial AI. "We see a lot of open sharing with users looking at different models related to machinery health in the open-source space. There are definite advantages for companies being open to sharing machinery-health data in multi-tenant cloud environments, because it helps us as an industry to better capture, understand and very quickly identify when there are systemic problems within pumps, sensors, PLCs or other elements," continues Hernandez. He also believes that the industry is becoming more comfortable with the ability to securely lock certain components of proprietary data within a platform, but still be able to share other selections of more generic data within a cloud environment. Facilitating and expediting this collaborative conversation will be key in accelerating the adoption and evolution of predictive machinery-health monitoring, which is among the more mature use cases for industrial AI, notes Hernandez.

Maintenance and optimization

One of the most prominent uses for industrial AI continues to be predictive maintenance. "Everybody's looking at how to get more throughput, and the easiest way to do that is to reduce your downtime with predictive maintenance," explains Clayton French, product owner — Digital Enterprise Labs at Siemens Industry. Siemens has worked with Sinopec Group's (Beijing, China; www.sinopecgroup.com) Qingdao Refinery using AI to investigate critical rotating-equipment components and predict potential causes of downtime. "We took six months of data and did a feasibility study, which found that eighteen hours before compressor failure, they would have been notified that the asset was having a problem, potentially saving around $300,000," says French. In another project, French notes that Siemens conducted a feasibility study in which AI was able to detect an equipment failure almost a month in advance. Such models integrate correlation analysis, pattern recognition, health monitoring and risk assessment, among others.

Furthermore, when an anomaly is detected, and a countermeasure is initiated in the plant to fix the problem, the AI can record the instance in its database. Then, the next time it senses that a similar failure is about to occur, the AI will recommend a similar countermeasure, which can reduce maintenance time in the long term. "This shows that the AI is learning and taking in all of these inputs. It continues to get better after its initial implementation," adds French.

Another maintenance example from AspenTech involves fouling in ethylene furnaces. "Typically, an operator will do periodic cleanouts of coke buildup on the furnaces, but what would be better is to get a better indication of when you actually need to

FIGURE 4. Open-source AI platforms enable experiments to be run remotely, bringing a new level of autonomous operations into chemistry laboratories

do a cleanout, versus just scheduling it. So what companies are doing is taking the relevant furnace operating data and being able to predict fouling to prevent unplanned downtime. Users can be sure they are cleaning out the furnace before a real operational issue occurs," notes Morse.

On the optimization side, she highlights a case where AspenTech helped a polyethylene producer to streamline transitions between product grades to maximize production value. As catalysts are changed out to accommodate different production slates, there is a transition period where the resulting product is an off-grade material. "The customer was able to apply an AI hybrid-model concept to look at how reactors are actually performing, and was able to decrease the amount of transition, both in terms of volume throughput, so they weren't wasting feedstock making a product they didn't want, but also by narrowing that transition time, they were also spending more reactor time making the preferred product instead of transition-grade material."

Rockwell Automation, Inc. (Milwaukee, Wis.; www.rockwell.com) has also done extensive work using AI to optimize catalyst yield and product selectivity in traditional polymerization processes, as well. "We started using pure neural networks to try to learn polymer reaction coefficients. We lean more and more into the actual reaction kinetics and the material balance around the reactors, trying to control the polymer chain length in the reactor. This is how you can get a specific property, such as melt flow or a melt index, on a polymer," says Pal Roach, oil and gas industry consultant at Rockwell Automation. In a particular example involving Chevron Phillips, an AI-driven advanced control model was applied to cut transition times between polymer grades by four hours. This change also led to a 50% reduction in product variability. In another case involving a distillation unit for long-chain alcohols, an AI-driven scheme applied to a nonlinear controller helped to cut energy consumption by around 35% and significantly reduce product-quality variability, as well as associated waste. "There are going to be more and more of these types of AI applications coming as the industry refocuses and transitions into greener energy and more environmental safety and governance consciousness," predicts Roach.

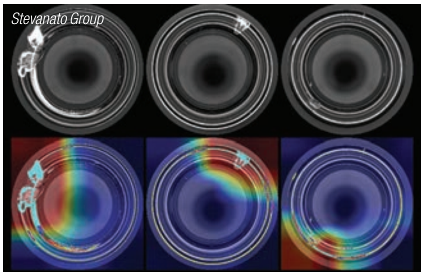


FIGURE 5. AI can be used to rapidly and accurately validate pharmaceutical products for defects, which reduces manual inspection requirements

Feedstock sustainability

As chemical manufacturers are increasingly looking toward more sustainable feedstock options, bio-based processes, such as fermentation, are reaching larger scales and necessitating more precise and predictive control. "We have used AI on corn-to-bioethanol fermentation optimization and seen yield increases from 2 to 5%, so that means you're getting more alcohol from the same amount of corn. And we've also seen overall production capacity increases as high as 20%," says Michael Tay, advanced analytics product manager at Rockwell Automation. To build the AI model for fermentation, Tay explained that Rockwell began with classic biofermentation modeling tuning the Michaelis-Menten equations, which predict the enzymatic rate of reaction, as the fundamental architecture. This enabled realtime control of the temperature profile in the fermenter. "You try to keep temperatures high, but then as alcohol concentration increases, you have to cool the reactor more so that the yeast gets more life out of it, because as the alcohol concentration goes up, the yeast performance goes down. The AI is showing dynamic recognition and adaptation of the fermentation profiles, so that's sort of the key to those yield improvements. But you're also getting more alcohol out of every batch," he adds. In addition to temperature-driven optimization, Rockwell has also used AI to improve the enzyme-dosing step in biofermentation processes. "If you have this causally correct model that is based on biological fundamentals, driven by data and AI, then you can optimize your batch yield to ultimately get more out of the yeast, which is your catalyst in the reactor," says Tay.

AspenTech is also working on developing accurate AI and simulation models for bio-based processes like fermentation, as well as looking at advanced chemical recycling models. "We're tuning those processes to be more efficient, and we're approaching predictability, but the feedstock variance will be something that we will be working on constantly," adds Paige Morse.

Reducing waste and emissions

While AI and other digital tools have historically targeted operational and financial objectives, many chemical companies are increasingly looking at process metrics that specifically consider environmental initiatives, such as reducing emissions and waste. Seeq worked with a CPI company to deploy an automated model of a sulfur oxides (SOx) detector's behavior during the time periods when its range was exceeded. Typically, accurate emissions reporting becomes more challenging when vent-stack analyzers "peg out" at their limits, necessitating complex, manual calculations and modeling. "Seeq's model development required event identification to isolate the data set for the time periods before, during and after a detector range exceedance occurred. Regression models were fit to the data before and after the exceedance, and then extrapolated forward and backward to generate a continuous modeled signal, which is used to calculate the maximum concentration of pollutant," says Buenemann. The solution also compiled relevant visualizations into a single auto-updating report displaying data for the most recent exceedance event alongside visualizations tracking year-to-date progression toward permit limits, which enabled the company to make proactive process adjustments based on the SOx emissions trajectory.

AI plays a major role in reducing waste by helping to ensure product quality, explains Mathworks' Rao, citing the example of Japanese films manufacturer Dexerials, which deployed an AI program for realtime detection of product defects. "A deep-learning-based machine-vision system extracts the properties of product defects, such as color, shape and texture, from images, and classifies according to the type of defects. The system was put in place to improve upon the manual inspection system, which was an error-ridden process with low accuracy. The AI system not only improved the accuracy, but also greatly reduced product and feedstock waste and frequent production stoppage."

New materials and products

Beyond improving day-to-day industrial operations, AI and ML technologies are also enabling advances in the synthesis of new materials and product formulations. In developing ML-powered digital technologies that encompass the chemical knowledge for synthetic processes and materials formulation, IBM (Armonk, N.Y.; www.ibm.com) took inspiration from sources very far removed from chemistry — image processing and language translation. "We learned that some of the technologies that have been developed for image processing were actually applicable in the context of materials formulation, so we took those concepts and brought them into the chemical space, allowing us to reduce the dimensionality of chemical problems," explains Teo Laino, distinguished researcher at IBM Research Europe. IBM is partnering with Evonik Industries AG (Essen, Germany; www.evonik.com) to apply such a scheme to aid in optimizing polymer formulations. "Quite often, when companies are working on formulating materials, such as polymers, the amount of data is relatively sparse compared to the dimensionality of the problem. The use of technologies that reduce the size of the problem means that there are fewer degrees of freedom, which are easier to match with available data. This is optimal, because users can make good use of data and can really see sensible benefits," he adds. Typically, optimizing a material to meet specific property requirements could take months, but IBM's platform for this inverse design process can significantly decrease that time, he says.

In designing a cognitive solution for chemical synthesis, IBM trained digital architectures that are normally

used for translating between languages to create a digital solution that can optimize synthetic routes for molecules (Figure 3). "By starting with technologies typically used for natural language processing, we recast the problem of predicting the chemical reactivity between molecules as a translation problem between different languages," explains Laino. Notably, the ML scheme has been validated in a large number of test cases, since IBM first made the platform (IBM RXN for chemistry, rxn.res.ibm.com) freely available online in 2018.

"We built a community of more than 25,000 users that have been using the models almost 4 million times. You can use our digital models for driving and programming commercial automation hardware, and you can run chemical synthesis from home wherever you have a web browser. It's a fantastic way of providing a work-from-home environment, even for experimental chemists," says Laino. IBM calls this technology IBM RoboRXN (Figure 4) and is using its ML synthesis capabilities for in-house research related to designing novel materials for atmospheric carbon-capture applications. IBM's ML platform has also been adopted by Diamond Light Source (Oxfordshire, U.K.; www.diamond.ac.uk), the U.K.'s national synchrotron science facility, to operate their fully autonomous chemical laboratory. "They are coupling their own automated lab hardware with IBM's predictive platform to drive their chemical-synthesis experiments," adds Laino.

AI and ML are also proving to be effective technologies for accelerating the product-development cycle. Dow Polyurethanes (Midland, Mich.; www.dow.com/polyurethanes) and Microsoft collaborated to create the Predictive Intelligence platform product formulation and development. The platform harnesses materials-science data captured from decades of formulations and experimental trials and applies AI and ML to rapidly develop optimal product formulations for customers, explains Alan Robinson, North America commercial vice president, Dow Polyurethanes. "Predictive Intelligence allows us to not only discover the chemistry and what a formulation needs to look like, but now we can also look at how we simulate trials. In the past, we'd be running numerous trials that take place over a period as long as 18 months, and now we can do that with a couple clicks of a button," says Robinson.

The demands of end-use polyurethane applications mean that finding the best chemistry for a particular product can be quite complex. "In a typical year we're releasing hundreds of new products, and in a typical formulation, there might be a dozen components that are individually mixed at different levels in different orders. We also have to think of all of the different tooling and equipment that the mate-

rials will be subject to, as well as the kinetics that have to be played out. So, the challenge was how to take all the kinetics, rheology and formulation data and create a system that could move us forward," explains Dave Parrillo, vice president R&D, Dow Industrial Intermediates & Infrastructure.

To build such a complex platform, Dow relied on theory-based neural networks that incorporated critical correlations for kinetics and rheology. "In a typical neural network, you feed it lots of data, which it learns from, and behind the scenes, it's tuning its knobs and weighing different influences. We can now influence those knobs with theoretical correlations so that the system not only learns, but gets smarter over time, and also starts to explore spaces where we might not have as much data. It folds theoretical, empirical, semi-empirical, and experimental information into a single tool," says Parrillo. One of the first major applications that Dow is trialing for the platform is polyurethane mattresses, with multiple applications to follow in 2022.

Once a product formulation is developed and manufacturing has begun, inspection and validation are key. Stevanato Group (Padua, Italy; www.stevanatogroup.com) recently launched an AI platform focused on visual inspection of biopharmaceutical products, looking at both particle and cosmetic defects (Figure 5). "AI can improve overall inspection performance in terms of detection rate and false rejection rate. AI can help to reduce false rejects and costly interventions to parameterize the machine during production," explains Raffaele Pace, engineering vice president of operations at Stevanato Group. Recently, trials of the automatic inspection platform have produced promising results, including the ability to reduce falsely rejected products tenfold, with up to 99.9% accuracy, using deep learning (DL) techniques. "Unlike traditional rule-based systems, DL models can generalize their predictions and be more flexible regarding variations," adds Pace. He also mentions that such advanced inspection performance can help to reduce the number of "gray" items, which are flagged on the production line but not rejected outright. Typically, such items require manual re-inspection, which adds time to the process. "This helps the entire process become more lean and have less waste, while maintaining and improving quality," he continues. The company is currently working to enhance detection accuracy for both liquid and lyophilized products, and also developing an initiative to create pre-trained neural networks that could then adapt to specific defects and drugs. "Producing such models will entail training the system with thousands of images," notes Pace. ■

Mary Page Bailey

Focus on Pumps

Minimize vibration and pipe hammer with these dampers

The new Equalizer Surge Dampeners — Integrated SD Series (ISD; photo) bolted metal option helps minimize vibration and control pipe hammer to protect the system piping and downstream instrumentation. The ISD Series dampeners are installed at the pump's discharge and have been specifically engineered to reduce fluid pressure and flow fluctuations for a smoother discharge flow. This function not only protects system equipment, but also helps extend the life, decrease the noise and increase the efficiency of this company's air-operated double-diaphragm (AODD) pumps. The new ISD Series stainless-steel metal dampeners are available in 25-, 38-, and 51-mm sizes. The bolted-construction design and PTFE, Buna backed, integral piston diaphragms offer maximum process fluid containment. — *Wilden, part of PSG, a Dover Company, Grand Terrace, Calif.*
www.psgdover.com/wilden

Wilden, part of PSG, A Dover Company

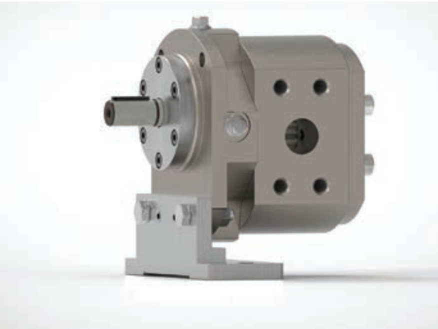
Avoid unplanned downtime with this monitoring system

Almost all of this company's pump series are now equipped with the i-ALERT 2 monitoring system as standard. Exceptions are made for individual designs, such as heated pumps, or if other monitoring systems are used at the user's request. The i-ALERT 2 sensor mounted on the bearing bracket (photo) monitors the vibration of the pump and the temperature of the bearings. If the pump exceeds the preset limits in two consecutive measurements, the unit goes into alarm mode. The i-ALERT 2 sensor transmits sensor-related data stored in the device (such as vibration, temperature, runtime information and device statistics) via Bluetooth to a free app. — *ITT Rheinhütte Pumpen GmbH, Wiesbaden, Germany*
www.rheinhuette.de

ITT Rheinhütte Pumpen

Small, magnetically driven gear pumps

Said to be the smallest pump series in the market, the DX Micro-Pump Series (photo) is suitable for dosing applications that demand low and precise flow capacities. These pumps can be configured with several component combinations to adapt to challenging process parameters and they come in three different sizes — 14/14, 14/8 and 14/4 — and are optimized for the required flow capacities and other process parameters. For example, the pump system can be configured with SSiC bearings, stainless-steel shafts, compact magnetic coupling and step-motor to manage 1 mPas fluid with discharge pressure of 25 bars and a small flowrate of 0.02 L/h. The DX 14 Series modular-build structure allows optimized combinations of bearings, shafts and seals depending on the application. — *Maag Pump Systems AG, Oberglatt, Switzerland*
www.maag.com



Maag Pump Systems

Pumps contribute to reducing CO_2 emissions from steel mills

Special pumps are needed to circulate the fermentation broth in LanzaTech's process that converts CO_2 into ethanol (photo). The major difficulties for the centrifugal and axial pumps are the high gas content combined with the requirement of avoiding the generation of large gas bubbles and the destruction of the microorganisms that are performing the fermentation. This company supplied pumps that are designed to provide a well-ventilated circulation of fluid while maintaining acceptable yields. The company has succeeded in manufacturing such pumps. A first installation in a Chinese steel mill near Beijing is running smoothly, and a second one for the ArcelorMittal group in Belgium is currently under construction. — *Emile Egger & Cie SA, Cressier, Switzerland*
www.eggerpumps.com

Emile Egger & Cie

Seal-less pumps in a larger capacity

The new Hydra-Cell Q330 Series pumps (photo, p. 20) feature a seal-less design to avoid the maintenance problems of mechanical or dynamic seals and packing that can leak and

Wanner Engineering

Atlas Copco Vacuum Solutions

Watson-Marlow Fluid Technology Group

Gather Industrie

wear. They are designed for a variety of high-capacity applications, including saltwater disposal (SWD), saltwater injection, bulk transfer and hydraulic lift in oil fields, as well as steam generation, reverse osmosis in water and wastewater treatment, mine dewatering, boiler feed and high-pressure cleaning. Models are available to meet API 674 performance standards, the company states. The new Q330 medium-pressure models offer flowrates up to 153 gal/min and a maximum pressure rating of 3,500 psi. New high-pressure models offer flowrates up to 118 gal/min and a maximum pressure rating of 4,500 psi. Hydra-Cell Q330 Series pumps can run dry without damage, will operate with a closed or blocked suction line, and can pump hot abrasive fluids effectively. The patented, seal-less Hydra-Cell Q330 Series pumps employ hydraulically-balanced, multiple diaphragms that enable the pump to handle high pressures with low stress and abrasive particulate matter up to 800 µm in size. — *Wanner Engineering, Inc., Minneapolis, Minn.*
www.hydra-cell.com

Dry, energy-saving vacuum pump for hygienic applications

The new oil-free DSS scroll vacuum pump (photo) is a robust, low-wear pump that is particularly suitable for vacuum generation in the rough vacuum range. A key feature of the innovation is its simple and effective operating principle for gas handling. Inside the pump there are two intermeshing, spiral-shaped screws made of aluminum. One spiral screw is fixed, while the second one rotates to compress the gas inclusions. The ergonomic vacuum pump is also characterized by low energy consumption, lower lifecycle costs and user-friendly operation, says the company. Due to the dry running of the pump, no oil changes are necessary. There is also no need to replace the exhaust filters, so the overall maintenance requirements are relatively low. The new pump is particularly suitable for applications in the pharmaceutical industry, as well as in food packaging and processing. — *Atlas Copco Vacuum Solutions, Cologne, Germany*
www.atlascopco.com

These metering pumps now offer four configurable outputs

Qdos chemical metering pumps (photo) now feature four configurable outputs to help users cut down on the need for additional PLCs and provide extra flexibility when communicating with SCADA or other external monitoring systems. The company has expanded its accurate and versatile Qdos Universal + Relay series to provide four configurable outputs, as well as the 4–20 mA. As a result, users can access increased options for connectivity, enabling improved communication regarding pump performance and function status. All Qdos Universal + Relay pumps produced after March 2020 feature four changeover relay outputs, with either 110 V a.c. 4-A, or 24 V d.c. 4-A contact rating. — *Watson-Marlow Fluid Technology Group, Falmouth, U.K.*
www.wmftg.com

A new gear pump for higher flowrates

This company has further developed its pump range with the introduction of the 3 series (photo). The new chemical process pump achieves flowrates of up to 4,000 L/h, with pressure differences of up to 10 bars. The pump is suitable for the delivery or metering of lubricating liquids and especially non-lubricating liquids, such as water, salt solutions, acids, alkalis and solvents. The use of the magnetic coupling, the internal cooling system, the high precision of the components and the double-volute construction of the pump housing result in a very robust design with an extremely long service life, says the manufacturer. Like all gear pumps from this company, the series 3 is clean-in-place (CIP) capable. — *Gather Industrie GmbH, Wülfrath, Germany*
www.gather-industrie.de

Vertical multistage inline pump for high-flow applications

The new CR 185 vertical multistage inline pump (photo, p. 21) is the latest addition to this company's CR range. Through advanced simulation-driven design, the CR 185 now delivers the most performance in its class — up to 1,275 gal/min and 1,230 ft of head. The CR 185 is suitable for high-flow water supply, water-transfer and water-treatment applications where energy efficiency is paramount. An improved impeller design reduces energy loss and the optimized flow path reduces pressure loss, both of which improve the pump's efficiency. On pumps up to 30 hp, the CR range features an integrated variable frequency drive (VFD),

the MLE motor, and for pumps larger than 30 hp, a panel-mounted CUE VFD is available to offer further energy optimization, efficiency and control. Low vibration reduces noise and ensures a longer lifespan. Additionally, balanced radial loads prevent shaft deflection that is common in single-stage pumps. A new thrust-handling device allows the use of standard motors on pumps with 100-hp motors and above. — *Grundfos Pumps Corp., Brookshire, Tex.*
www.grundfos.us

Pump motor system offers all-in-one drive solution

The ID300 Fusion Integrated Motor Drive (photo) features U.S. Motors brand 1–10-hp UL-certified induction motors and customizable variable speed drives. With this compact all-in-one product, original equipment manufacturers (OEMs) do not need to buy standalone products, such as motors, drives, conduits and cords, and integrate them for a user application. The ID300 Fusion incorporates all of the functions of a VFD into the motor for better system performance and efficiency. The integrated ID300 Fusion provides superior control and monitoring capabilities that help with realtime pump management and intelligent analytics. With pumping applications in mind, the ID300 Fusion allows OEMs to embed the pump curve information into the drive so that the pump runs at its best efficiency point without an external sensor. That saves the cost of the sensor, the labor to install it, and also minimizes the risk of error if the drive is incorrectly programmed for the sensor. An onboard programmable logic controller (PLC) can regulate the pressure (constant pressure/variable flow). When programmed with the pump curve, the ID300 PLC can perform sensor-less constant pressure control, eliminating sensor cost and simplifying its installation and commissioning. One ID300 Fusion can control up to three additional constant-speed backup pumps. — *Nidec Motor Corp., St. Louis, Mo.*
www.nidec-motor.com

A solenoid pump for fluid control

The SSDP (photo) is a miniature fixed-displacement solenoid pump said to be highly accurate and reliable with few moving parts, making it an ideal replacement for inferior and more-costly diaphragm and peristaltic pumps. The SSDP works like an automatic syringe. An internal diaphragm uses minimal power to draw media into the device when energized and expels and seals off flow when deactivated, eliminating the need for an external shut-off valve. This process is repeated to deliver the necessary amount of media based on the application requirement. The pump is capable of self-priming when located up to 3 m above its fluid reservoir. Manual priming is also possible. — *Spartan Scientific, a div. of Canfield Industries, Youngstown, Ohio*
www.spartanscientific.com ■

Gerald Ondrey

Grundfos Pumps

Nidec Motor

Spartan Scientific

Timmer

Coval Vacuum Technology

ONLINE ONLY

Live monitoring of pumps with this IoT solution

The tim IOT digital solution (photo) enables location-independent, real-time monitoring and predictive maintenance, even for purely mechanical pumps. Scheduled to launch this month, tim IOT consists of a retrofittable sensor for data acquisition and the tim IOT smartbox, which connects the pump with the tim IOT cloud platform. Operators benefit from, among other things, a significantly higher process reliability, a minimization of downtimes and considerable cost savings due to better planning, says the company. The system design of tim IOT is quite simple: The pump must first be equipped with an intelligent sensor. This sensor is already integrated as standard in most of this company's double diaphragm pumps. The sensor is then linked to the tim IOT smartbox, which transmits the data to the cloud by means of a secure transmission, for example via a separate LTE router that is independent of the company network. The visualization and evaluation of the data is done on freely selectable end devices such as PCs, smartphones or tablets. Clearly structured histograms, tables and statistics can be viewed from any location. In the case of error status or exceeding set values, a notification in the IoT platform or to a defined email address is made. Parameters such as pump frequency, number of strokes or pressure curves are permanently visible. Predictions on wear and tear, as well as the planning of repair measures, become much more precise — this ensures optimum use of the pumps over their entire lifetime. — *Timmer GmbH, Neuenkirchen, Germany*
www.timmer.de

Wear/abrasion-resistant pump components improve reliability

WR (Wear Resistant) and AR (Abrasion Resistant) pump components are engineered from high-performance thermoplastic composite materials for centrifugal and magnetic-drive pumps. These composites are available in a variety of materials, temperature ranges and operating pressures to meet pump requirements for energy production, water, wastewater and chemical applications. The WR line offers excellent wear and friction properties, along with superior non-galling and non-seizing performance. Offering extended dry-run performance and exceptional chemical resistance, the WR materials can often reduce running clearances by more than 50%, says the company. The AR composites are a recommended abrasion-resistant solution when pumping in a watery media with the presence of abrasive materials like sand or sludge. Both WR and AR composites last up to five times longer than traditional materials for dramatically longer lifetimes, as well as reduced downtime and reduced maintenance requirements, says the company. — *Greene, Tweed & Co., Lansdale, Pa.*
www.gtweed.com

Vacuum pumps for handling systems

Vacuum handling systems in industry must respond to very diverse requirements, gripping parts of different weight or material, integration on machines and robots or high-speed operation. The GVMAX HD series of vacuum pumps (photo) combine robustness, power, modularity and communication, allowing them to adapt to multiple applications. The IO-Link communication interface of the pumps makes installation fast and economical, supports continuous diagnostics, centralized parametrization and efficient communication with higher-level protocols, including Ethernet/IP, Profinet and EtherCAT. In addition, thanks to the NFC technology integrated in the GVMAX HD vacuum pumps, all parametrization and diagnostic functions are accessible and can be modified in the dedicated Vacuum Manager application (app) on an Android or IOS mobile device. — *Coval Vacuum Technology Inc., Raleigh, N.C.*
www.coval.com

NFPA 652 and Dust Hazards Analyses

Department Editor: Scott Jenkins

The National Fire Protection Association's (NFPA; Quincy, Mass.; www.nfpa.org) NFPA 652 (Standard on the Fundamentals of Combustible Dust) creates a single, unified combustible-dust standard that applies to "all facilities and operations that manufacture, process, blend, convey, repackage, generate, or handle combustible dusts or combustible particulate solids." This one-page reference provides information on the NFPA 652 standard and the requirements for conducting a dust-hazard analysis (DHA).

Dust sampling

NFPA 652 includes procedures that all facilities can follow to identify areas where potential combustible-dust hazards exist (Figure 1). An initial step involves collecting dust samples from throughout the facility to determine the combustible or potentially explosive qualities of the dust.

A sampling plan should include the following elements:

- Identification of locations where fine particulate materials and dusts exist
- Collection of representative samples
- Methods to ensure preservation of sample integrity
- Communication with the test laboratory regarding proper sample-handling procedures
- Documentation of samples taken
- Safe sample-collection practices

Following a rigorous sampling plan helps facility operators ensure that the dust samples are accurately analyzed to determine their combustibility.

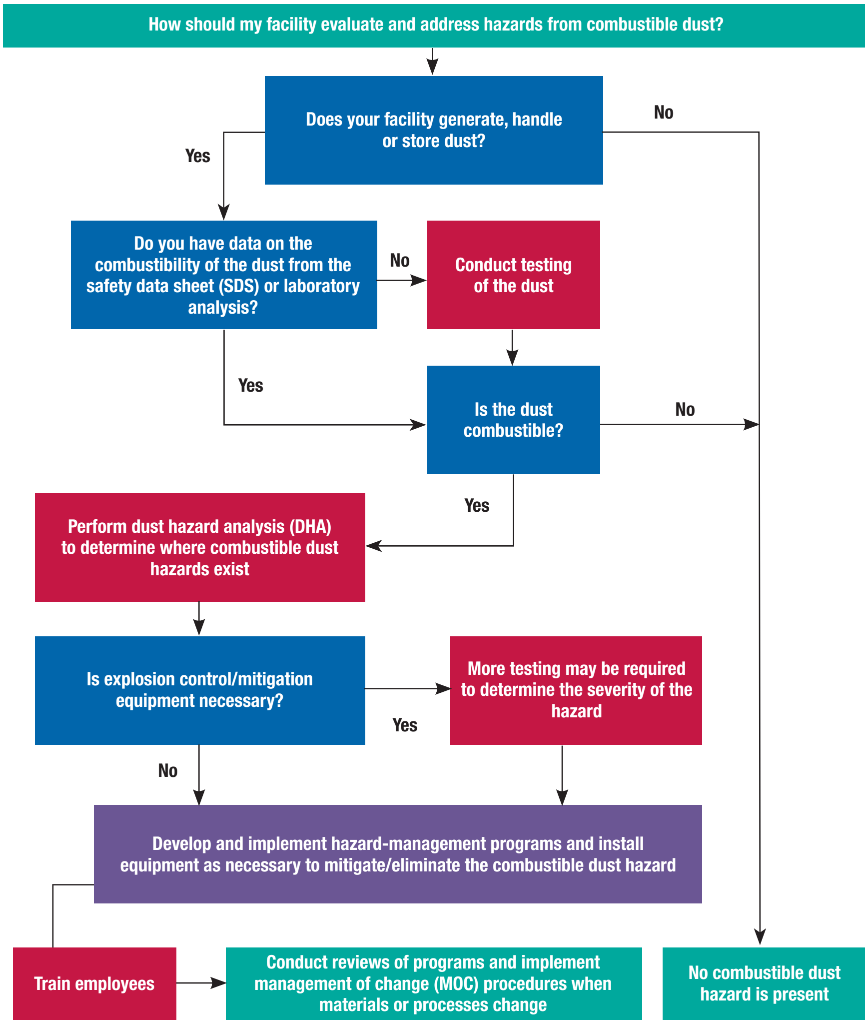


FIGURE 1. Evaluation of potentially combustible dusts at a facility involves sampling materials and conducting a dust hazards analysis

Conducting a DHA

For any materials identified as being combustible or potentially explosive, the facility should complete a DHA to evaluate the potential hazards associated with a fire or explosion due to the handling of the materials throughout the facility. Inspections of areas where combustible dust is handled also allow facility operators to develop recommendations to minimize the risks of a combustible-dust incident.

Specifically, a DHA should include the following:

- Identify and evaluate locations or processes throughout the facility where potential fire, flash fire or explosion hazards exist
- Identify and evaluate specific fire and deflagration scenarios where fire and explosion hazards exist
- Identify safe operating ranges
- Identify safeguards in place to mitigate the hazards of a fire or explosion
- Recommend additional safeguards where needed

The DHA must be completed or led by a qualified person who has demonstrated the ability to understand combustible dust and associated hazards through education or experience. This person should inspect all buildings and processes, understand the properties of the potentially combustible dusts present, identify all potential ignition sources, and evaluate the effectiveness of any deflagration-suppression or protection systems that are currently in place.

Taking action

Once a DHA is complete, facilities should work to mitigate combustible dust hazards by both preventing fugitive dust from being discharged from equipment and by installing an effective dust-collection system. The facility should monitor dust hazards and provide training on combustible dusts, including general and job-specific training. ■

Editor's note: the material in this column of "Facts at your Fingertips" is adapted from the following article: Frendahl, C., Edwards B. and Davis, J. NFPA 652: Standardizing Combustible Dust Standards, *Chem. Eng.*, May 2016, pp. 74–78.

Production of Sodium Hydroxide from Brine

By Intratec Solutions

Sodium hydroxide (NaOH) is a white, translucent crystalline solid that is widely used in the chemical process industries (CPI). NaOH is often referred to as caustic soda, due to its corrosive action on many substances: it decomposes proteins at room temperatures and may cause chemical burns to human bodies. Although it does not occur in nature, NaOH has been manufactured at large scale for many years from readily obtainable raw materials and is used in numerous industrial processes (Figure 1).

Sodium hydroxide is mainly used in pulp and paper manufacturing, alumina extraction from bauxite in aluminum production, as well as in the textiles industry and drinking water production. NaOH is also an important compound in the manufacture of soaps and detergents, in waste gases scrubbing, saponification and etherification and esterfication reactions; as well as in basic catalysis.

Pure NaOH has a high affinity for water and may form hydrates depending on the concentration. Since some hydrates have melting points greater than 0°C, insulation or heating during storage and transportation considerations may be required. Additional care is required because in the presence of moisture, NaOH readily reacts with atmospheric carbon dioxide to form sodium carbonate. Shipping NaOH can be accomplished in steel drums for concentrations up to 50%. For higher concentrations, pure nickel drums are required due to corrosion effects.

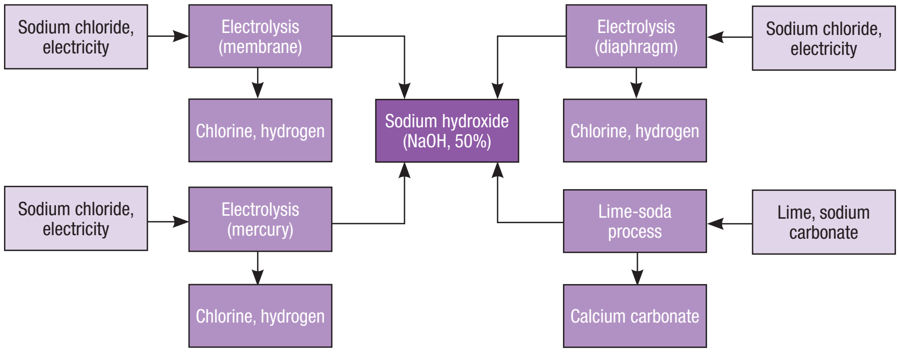


FIGURE 1. Several processes involving the electrolysis of salt brine, along with one using lime soda and sodium carbonate, can be used to produce sodium hydroxide

NaOH production process

The production of NaOH from sodium chloride (NaCl) comprises three major sections: (1) brine purification; (2) electrolysis; and (3) product recovery (Figure 2).

Brine purification. Initially, recycled depleted brine is mixed with water and re-saturated with fresh NaCl. Heavy metal ions (for example, Ca^{2+} and Mg^{2+}) present in the brine would be harmful to the membranes. So the brine is treated with precipitants in such a way that the metals precipitate, forming a sludge, which is removed by settling in a clarifier. Subsequently, the clarified solution is filtered and then purified by ion-exchange resins to remove residual hardness and achieve acceptable levels.

Electrolysis. The ultrapure brine and electricity are the main inputs to the electrolysis area. The brine is fed into the anolyte compartments of the cells, separated from the catholyte by cation-exchange membranes. Chlorine gas is generated at the anodes and sodium ions migrate through the membranes into the catholytes. The depleted brine from the anode compartments is dechlorinated downstream and then returned to the brine saturation stage. On the catholyte side, water is electrolyzed, generating hydrogen gas and hydroxyl ions. The membranes prevent the migration of such hydroxyl ions into the anolytes in such a way that hydroxyl ions combine with the sodium ions, forming caustic soda. The addition of demineralized water keeps the catholytes concentration at the desired level.

Products recovery. Hydrogen from the electrolysis process is compressed and directed to consumers. The caustic soda solution is concentrated to a saturated 50 wt.% NaOH solution — the commercialized form. The chlorine gas produced is sent to a drying system, consisting of drying towers, where concentrated sulfuric acid circulates as a dehydrating agent. The dry chlorine gas is compressed and then liquefied before being send to storage vessels. ■

Edited by Scott Jenkins

Editor's note: Content for this column was originally developed by Intratec Solutions LLC (Houston; www.intratec.us) and is edited by *Chemical Engineering*. The analyses presented are based on publicly available and non-confidential information. The content represents the opinions of Intratec only. More information about the methodology for preparing the analyses can be found, along with terms of use, at www.intratec.us/che.

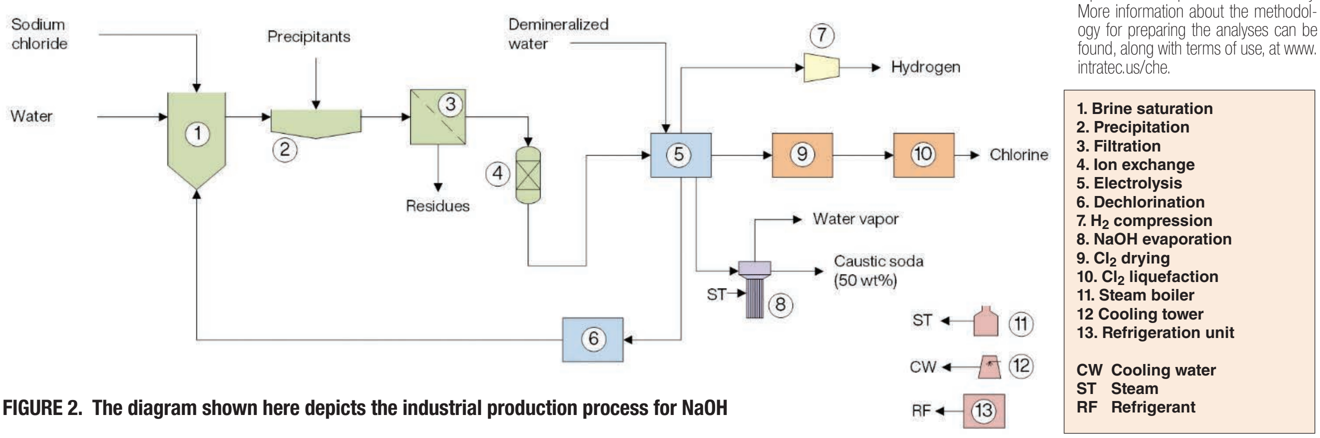


FIGURE 2. The diagram shown here depicts the industrial production process for NaOH

Process Analytical Technology Advances

Developments in laser technology and significantly increased computing power are making process analyzers available for new applications and even for closed-loop control

Wolfgang Lubcke
Endress+Hauser

IN BRIEF

Process analytical technology (PAT) has undergone rapid development in recent years. Further developments in laser technology, the miniaturization of optical and electronic components and the implementation of complex chemometrics models (Figure 1) now enable novel and robust field instruments that can analyze even diverse mixtures of substances in a highly selective manner.

This article presents an overview of PAT, and describes some of the applications and benefits of these technologies. It also addresses some of the misconceptions about cost and reliability issues.

Introduction to PAT

I wonder if Paul Gmelin had any idea of the success story he had initiated in the chemical process industries (CPI). At the beginning of the 20th century, the workers in the physical laboratory of the Badische Anilin- und Soda Fabrik (BASF) in Ludwigshafen, Germany, was faced with a major challenge: During experiments on ammonia synthesis, it became apparent that the large gas flows had to be monitored in terms of their composition. Gmelin then developed the so-called pipe analyzer. Using online analysis, this analyzer made it possible to measure the ratio of the nitrogen and hydrogen gases during the synthesis, and thus control the ammonia production process.

In 1913, Gmelin received a patent for his pipe analyzer — and modern PAT was born. After that, PAT slowly but surely began its triumphant advance. This is because PAT can be used to measure chemical properties, the composition of mixtures, their concentrations and their desired or undesired changes. PAT therefore brings the laboratory to the process, and offers decisive advantages over offline analysis. This is because traditional offline quality control requires that samples have to be taken and transported to a quality laboratory for analysis. Several hours may pass before the results become available, and this delay prevents results-based process control. PAT delivers results in or near real time. As a result, PAT enables continuous monitoring of production processes, as well as an optimized, target-product-oriented production.

Over the years, PAT has become more and more an established discipline, and is now widely used throughout the CPI. Today, PAT encompasses more than 80 different measuring methods that are used on liquids, solids and gases (see Table 1 for a small selection). Just to clarify, "analytical technology" is a term that refers to both laboratory analysis and process analysis, whereas PAT refers to process analysis. The spectrum ranges from simple measurement methods, such as conductivity, viscosity and pH, through photometry, paramagnetic

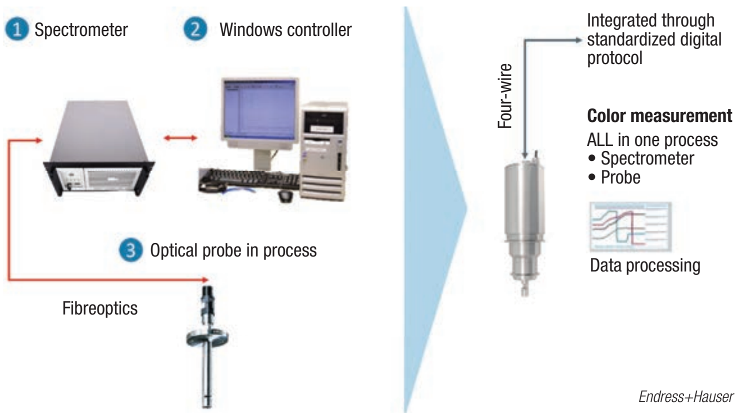


FIGURE 1. Thanks to technology advances, the complexity of analytical instruments is being reduced. Color measurements, for example, can now be performed with the compact field device (right) that contains everything — spectrometer, probe and electronics for data processing

oxygen measurement and diode-laser spectroscopy (DLS), to new complex methods, such as Raman and ultraviolet (UV) spectroscopy.

Process analysis works in several different ways (Figure 2): inline, with sensors directly in the vessel or in the pipeline; online, with the associated automatic sampling and sample preparation; and at-line, with sequential sampling.

The requirements for process analysis, especially in the CPI, are clear and diverse: they should be able to map the process and be used safely in hazardous areas, in harsh environments and in complex media. Due to the fluctuation in the composition of the media, a high level of robustness and selectivity of the process analytics is required. Maintenance should also be as simple as possible. Standardized interfaces for data transmission to process control systems are needed. The goals of using PAT in the CPI are an optimized increase in yield, the capacity of the plant or the reduction of energy or labor costs.

In the past, spectroscopic methods in particular were often not fast enough, too error prone for harsh process environments or not powerful enough. However, advances in laser technology, significant microcomputer power and the implementation of complex chemometrics models now enable novel and robust field devices that can analyze even diverse mixtures of substances highly selectively and reduce complexity for the user. Such devices make it possible to increasingly utilize quality-relevant measurements and analyses from the laboratory to inline and online measurements during production.

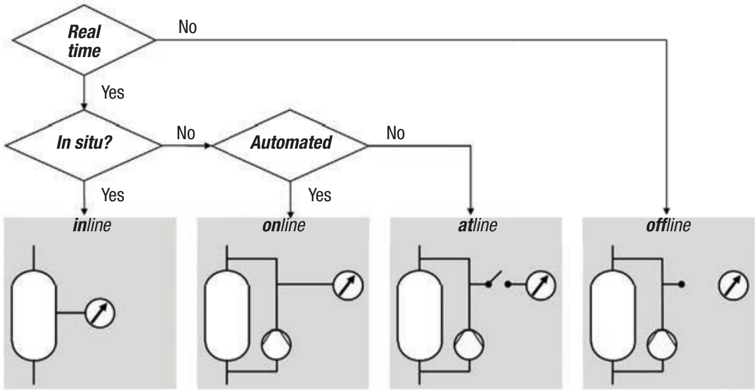


FIGURE 2. These diagrams, which show typical arrangements for analyzers (bottom) and a decision tree for classifying the analyzers to (top), help clarify the nomenclature for PAT applications (Adapted from Ref. 1, with permission)

For the CPI, this ongoing industrialization of laboratory technologies opens up a wide range of opportunities. With the use of PAT, it is currently possible to achieve higher added value than ever before.

Trends in process analysis

In recent years, great progress has particularly been seen in Raman technology. The laser-based method can analyze gases, solids and liquids down to the level of molecules. Raman spectroscopy is based on the interaction of an incident, monochromatic light beam with the matter under study. Individual photons transfer some of their energy to the molecules, but the molecules can also transfer energy to individual photons in reverse. This light scattering produces a fingerprint-like pattern for each substance that provides information about the composition and nature of the material. In the laboratory, Raman spectroscopy has already proven its worth for complex substances analyses, and commercial Raman systems are now available in robust, reliable inline process solutions. Raman technology offers the possibility of measurement through glass reactor walls or windows.

Due to fast signal processing, measured values are available within 15 seconds (at best; see Table 2) and therefore ensure multiparameter analysis in real time. This sometimes brings decisive advantages in complex chemical processes. Thanks to precise knowledge of the mixture, the process can be optimally controlled, thus reducing raw material and energy consumption. In the production of synthetic rubber, for example, the determination of quality

TABLE 1. A SELECTION OF PAT DEVICES FOR MEASURING DIFFERENT PARAMETERS

LIQUIDS

Color	Composition	Concentration	Conductivity	Density	Disinfection	Metals Nutrients	Oxygen Dissolved	pH ORP	Sum parameter	Turbidity	Viscosity
Photometer	Raman	Ultrasonic	Conductive	Resonance	Chlorine	Colorimetric	Amperomet	Glass	Colorimetric	Absorption	Torque
Spectrometer	IR-Absorption	Resonance	Inductive	Radiometric			Optical	Isfet		Scattering	

GASES

Composition	Concentration	Density	Oxygen
Raman	TDL-AS 1)	MEMS 2)	QF 3)

SOLIDS

Composition	Moisture
Raman	TDR 4)

Notes:
1) TDL-AS = Tunable-diode laser absorption spectroscopy
2) MEMS = Micro-mechanical electrical system
3) QF = Quench fluorescence
4) TDR = Time-domain reflectometry

Reaction monitoring of fermentation

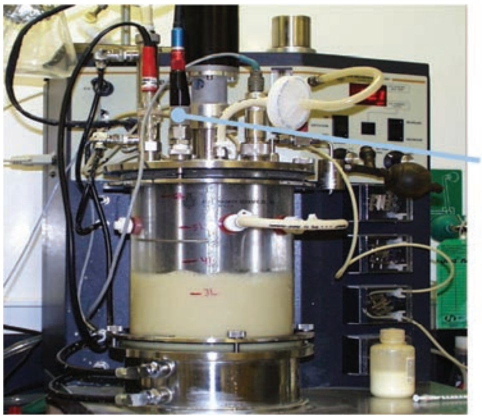


FIGURE 3. With a single Raman probe it is possible to monitor — in real time — concentrations of glucose and metabolites during a fermentation process

parameters, such as polymer structure and residual monomer content, minimizes waste. Raman spectroscopy can also be used to monitor the production and processing of synthesis gas (syngas; H_2 + CO) to generate ammonia or urea, and thus significantly increase yields. New possibilities are also opening up in the life sciences sector, for example in controlling cell growth in bioreactors. Here, the precise determination of the concentrations of glucose and metabolites is important, among other things (Figure 3). Thanks to inline measurement, laboratory release can be replaced by realtime release, so batches no longer have to be held back for days. The monitoring of a distillation process is another important application of Raman spectroscopy (Figure 4).

Decisive further developments also characterize ultraviolet/visible (UV/VIS) and near infrared (NIR) spectrometry. Here, the trend is moving from online to inline measurement due to technical innovations. With inline spectrometers, measurement times in the range of seconds can be achieved, and thus advanced process control can be realized. In addition, the reduced complexity of the instruments leads to a broader range of applications. Until now, the sensitive spectrometers had to be located outside the process and connected to the measuring probes via a fiber-optic cable. Innovative inline spectrometers now integrate the previously separate measurement-probe components, via fiber-optic cable and sensor, into compact and robust devices. This enables them to be directly installed in the process and integrated into the process-control system (See Table 2 for a comparison of Raman and NIR).

Now that such devices are easier to use, even more plant operators can benefit from the high precision of the spectrometers, for example, in the color analysis of products. Unlike photometers, which operate at only one or multiple wavelengths, these new process spectrometers measure throughout the entire visible range (UV/VIS wavelength ranges from about 200 to 750 nm), and thus the entire color spectrum is covered. The wavelength range of NIR (about 700–3,000 nm) complements the color spectrum, and is capable of exciting molecular vibrations. From the reflected spectra, information about molecular composition can be determined. NIR can be used for both identification and quantification of substances. NIR spectroscopy can therefore be widely used in chemical analysis, for example, to determine water content in feedstocks or products being dried, as well as for quality control and process control.

There have also been further developments in the measuring of moisture in solids and the concentration of liquid solutions. Time-domain reflectometry with intelligent micromodule elements (TRIME-TDR) is increasingly being used for moisture measurement. This special variant of radar time-of-flight measurement is a highly accurate and reliable online "high-tech" measurement technique. In this method, a pulse is generated that travels along a conductor and is reflected. The transit time of the pulse is directly related to the water content or moisture in a material. In contrast to other technologies, the conductivity has no impact on the measurement. As a result, a high accuracy is possible.

For concentration measurements in liquid process media, new systems are available for realtime online measurement that work with surface acoustic waves. These are high-frequency sound waves that can be compared in their physical behavior to seismic waves, such as those that occur in earthquakes. By evaluating the transit time and wave amplitude, acoustic parameters of the liquid, such as the speed of sound, the impedance and the density can be determined, and from this information, concentration can be derived precisely and quickly. Because the system has no moving parts, there is no wear and maintenance is low.

If we consider the area of quality monitoring of feed gases, tunable diode-laser absorption spectroscopy (TDLAS) is gaining in importance, compared to alternative methods, such as gas chromatography (GC). Modern online TDLAS analyzers selectively measure impurities, such as ammonia, moisture or acetylene, with high precision, even at concentrations below 1 part per million (ppm). The analyzers provide reliable measurements within seconds, enabling fast action. They help improve process control, meet product specifications, avoid catalyst poisoning and minimize the need for flaring.

Costs versus benefits

The preceding overview of the advances in PAT shows that its utility is great in all steps of the production process, from feedstock analytics, in-process analytics and product analytics. PAT devices can be used to monitor feedstock purity and catalyst concentration, and to adjust stoichiometry in reaction vessels. Concentration and state data from the process allow an improved understanding of the process via correlation analysis. The rapidly available PAT readings allow improved process control and even realtime process control.

Thus, the use of PAT leads to a higher degree of conversion and end-point-controlled processes. Faulty batches and the associated waste of unusable product are avoided and byproducts reduced. Yield is increased, product quality is improved,

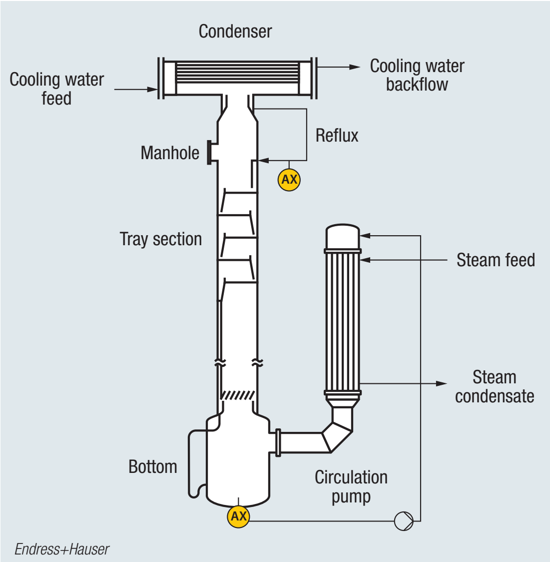


FIGURE 4. With multi-point Raman probes (AX) strategically placed in a distillation process, it is possible to perform sampling-free process monitoring. The technology is capable of distinguishing among isomers, for example

the manufacturing process is optimized, and energy and reactants are saved. Plant capacity and availability are increased.

However, there are also reservations about the use of PAT. One reason is that the costs of PAT are often overestimated and the benefits massively underestimated. The most common objection from the CPI is: "But PAT is very expensive, isn't it?" Indeed, at first glance, the investment costs appear to be high. This is because PAT is produced in relatively small quantities. Moreover, PAT solutions are always tailor-made solutions that have to be individually adapted to the specific process and the user's requirements. A PAT system is a system consisting of sensor or sampling or sample preparation, analyzer, sample recirculation or sample disposal. If necessary, additional equipment, such as a calibration device, may also be added. As with all investment decisions, however, the benefits of a process-analysis measuring station must be clear from the beginning and the outlay must be in reasonable proportion. In addition, different measuring principles and designs should always be considered.

Then there is the question of maintenance costs: "Aren't these also high?" Here too, the answer is "yes." Although there have been strong advances in manageability and robustness, PAT systems actually have a higher maintenance cost that other field devices for measuring non-specific variables, such as temperature, pressure, flow and level. Because many process analyzers are more complex, receive more mechanical components and sensitive parts, maintenance accounts for an average of 5 to 10% of the total cost (capital expenditures; CAPEX) of the measuring point. However, the expense can be reduced in advance by setting up the analytical measuring point to meet the requirements. It is then the task of the analytical engineer to select durable, low-maintenance sensors or to design a customized sampling system with, for example, correctly dimensioned filters, separators and the appropriate materials of construction.

The first PAT devices, such as TDLAS or Raman analyzers, also already have diagnostic, verification and self-monitoring functions. The intelligent technology of modern sensors makes it possible to evaluate numerous sensor signals already in the device.

Standardized diagnostic messages with clear instructions for action enable condition-based maintenance here. The permanent self-diagnosis of the device guarantees safe plant operation with extended test cycles. A guided sequence for device verification without interrupting the process generates unambiguous test results. The automatically generated test protocols support verification in accordance with industry- or country-specific regulations, laws and standards. The monitoring functions allow the implementation of predictive maintenance concepts through trend detection.

Data-based decisions are also supported by intelligent sensor technology, which is now widely used. Such intelligent sensor technology not only digitizes the measured analog values of inline liquid analysis (for example, pH, redox) in the sensor itself, but also reports signal transmission faults and facilitates the replacement of pre-calibrated sensors. Associated software stores all sensor and calibration data. Maintenance and calibration cycles are then no longer processed according to a fixed SOP (standard operating procedure) based on empirical values, but can be planned as required, as the load status of each individual sensor is known.

Expenses can also be reduced by risk-based maintenance. Generally speaking, if planned according to requirements and maintained properly, the availability of analytical measuring points is now so good that they can be used in safety facilities and in the quality control area. Realtime batch release with quality-relevant analytical measuring systems is also not a problem.

On closer inspection, however, it quickly becomes clear the questions "Isn't PAT very expensive after all" and "Aren't maintenance costs high?" can be answered with a "yes, but..." This is because replacing tedious laboratory analysis with fast process analysis is worthwhile. Even if the initial costs are high, the return on investment (ROI) is often only a few months.

Examples of PAT applications

The following real-life examples impressively show the impact PAT has as a "window into the process" compared to laboratory analysis, and how economical knowledge-based production is made possible with PAT. They were recorded by the International User Association of Automation Technology in Process Industries (NAMUR; Leverkusen, Germany; www.namur.net.en) [2]. Additional examples are given in Table 3.

Ingredient analysis. In the past, the quality and optimum composition of the components in the inlet stream of a plant was determined every 2 h by a 40-min laboratory analysis. This practice was replaced by online Raman spectroscopy with a measuring probe. Since then, the mea-

TABLE 2. A COMPARISON OF NIR AND RAMAN SPECTROSCOPY PERFORMANCE

	(FT)-NIR in-line: Absorption	Raman in-line: Scattering – Emission
Technical data		
LOD/LDL*	>100 ppm	>200 ppm
LQL*	>200 ppm	>2,000 ppm
Up-date time	5 s [simple molecules] – 4 min [complex]	15 s [simple molecules] – 30 min [complex]
Qualitative comparison		
Similar benefits	One probe measures a large variety of molecules – small and complex at the same time	
Unique benefit	• Well established technology with publicly available application knowledge • Faster in response – high-precision measurement in approximately 1 min • Less expensive especially hardware OPEX • Easier EX-conformity	• Primary measuring effect – easier signal processing • Analysis of both solid and liquid phase in suspensions • Very sensitive to isomers, for example, cis/trans in double bonds, *n-/iso-* in C chains, *o-/m-/p-* in aromatics, polymorphs in solids • Less efforts for "model maintenance" and simpler transfer to different hardware platforms
Grey zone	• Insertion, transmission and transflexion probes (5–10 mm gap)	• Challenging below 1,000 ppm • Fluorescence (993 nm)
Limits	• Aqueous processes can be challenging if analytes are at low concentration	• For example, ammonium <1 g/L

Notes: LOD = limit of detection; LDL = lower detection limit; LQL = lower quantifiable limit

surement is carried out every 3 min during the process. This quickly led to the prevention of off-specification production. If the reduction in laboratory analysis, the purchase and installation of the measuring equipment, the depreciation of the device and the annual support costs are calculated against the preventive off-specification production, the return on investment was 6 mo.

In-process analysis. Online Raman spectroscopy with a measuring probe measures chlorination every 3 min in a batch process. With PAT, laboratory analysis was saved several times per batch, the cycle frequency of the plant was increased and a capacity increase of around 10% was achieved. The reduction in laboratory analysis, the purchase and installation of the measuring equipment, the depreciation of the device and the annual support costs, as well as the capacity increase, also resulted in a ROI of 6 mo.

Release analysis. For residual moisture measurement of a product after drying and before packaging, laboratory analysis was very simple, but also very lengthy at 120 min. Online NIR spectroscopy with up to six measuring heads now determines the

residual moisture every 12 min. This makes it possible to quickly detect a product that does not meet specifications. The real advantage, however, lies in the compliance with specification limits. As a rule, specifications are significantly undercut without the use of online measuring equipment in order to prevent rejection by the customer in any case. By exploiting the specification limit, the ROI can now be seen as less than 6 mo., depending on the product price. In addition, energy costs and the associated CO_2 emissions are reduced.

TABLE 3. A SELECTION OF PAT APPLICATIONS

Example measurement task	Operating principle	Main parameter drivers	Investment	ROI
Reactor monitoring for catalyst poison	Thermal conductivity measurement	Process improvement and reduction of H_2 losses	€120,000	3 months
Online monitoring of the equilibrium concentration of various carboxylic acids	Near infrared (NIR) spectroscopy	Stabilization of a crystallization process	€675,000	12 months
Distillation monitoring for feed control	NIR spectroscopy	Process improvement through automated column control	€350,000	6–12 months
Residual moisture determination of a powder	Microwave absorption	Reduction of drying time and improvement of product quality	€50,000	24 months
CO smoldering fire detection	Nondispersive IR	Process safety	€200,000	Risk-reduction
End product control	NIR spectroscopy	Product release possible at any time without laboratory measurement	€350,000	12 months
Monitoring of inrush of current for process control	Raman spectroscopy	Prevent off-specification production due to waiting time for laboratory values	€300,000	6 months

Source: Ref. 2, with permission. Date: October 30, 2017

These examples all refer to online methods. By eliminating the need for sampling and sample preparation for analysis, inline methods once again ensure lower costs and significantly increased operational reliability with comparable measurement accuracy. For example, inline Raman spectroscopy has been successfully used in urea synthesis to optimize process parameters. The productivity of the plant, which has an annual output of 495,000 tons, was increased by 0.5% as a result. The higher yield from process optimization alone, as well as the savings in energy consumption and emissions, add up to €700,000 to 800,000 annually.

Another question that also arises in the decision-making process is "When should one continue to rely on laboratory analytical analysis, and when to rely on PAT?" The advantages of an analytical laboratory lie in its flexibility. With the appropriate analytical equipment and experienced laboratory technicians, analyses that are not part of the daily routine can also be carried out there. However, apart from extremely time-consuming sample preparation and special analyses, it makes more sense to automate routine analyses.

According to NAMUR, the following rule of thumb applies. From around one analysis per day, process analytics is less expensive than laboratory analytics. Further advantages are that process analytics also provide measurement results over the weekend and holidays without shift work. Current measured values are available without any major delay, and only this allows them to be used in process control systems. And sample falsification due to sampling errors is ruled out. The main disadvantage of offline analysis is also the limited number of samples, the often-necessary personal protection during manual sampling, the possible alteration of the sample from sampling to analysis and the long time usually required to obtain the analysis result and return it to the process.

The future is digitalization

The potential of PAT is far from being exhausted. In addition to technological developments in the instruments themselves, the digital transformation, which is noticeable in all areas, will influence PAT in the future and lead to new fields of application and changes in work flow. As a result, PAT will make production processes even more economical, cost effective and flexible in the future.

In general, digitalization aims to leverage the huge data potential in the field that has been lying fallow up to now. Measured values from field devices and process analyzers, as well as other information about devices, analyzers and the process should be able to be read out and transferred for applications beyond the actual measurement, control and regulation tasks. The data, which have been made accessible via internet technologies, are then to be used through systematic evaluation, comparison, enrichment or linking. Linking device and process parameters thus once again creates the basis for targeted process optimization. The processing of large volumes of data in the cloud with the aid of intelligent algorithms forms the prerequisites for the new digital services and business models.

For starters, the use of data for Industry 4.0 concepts in operation and maintenance is envisaged. The long-term goal is networked sensors, which in turn are the prerequisites of cyberphysical production systems (CPPS) and future automation concepts for the CPI. Work is also being done on virtual sensors in this context. The aim here is to correlate various parameters measured by real sensors and thus determine further parameters that cannot otherwise be recorded directly.

Such applications raise the question of how the measured values of the field devices and other information can actually be transmitted. One approach is to export the data via open interfaces, such as OPC UA. This is a technology generation of the OPC Foundation for secure, reliable and manufacturer-independent transport of raw data and preprocessed information. The actual automation of the plant according to the classic pyramid should remain largely unchanged, thus ensuring

plant safety. For Industry 4.0 concepts in operation and maintenance, the field devices are accessed via a second communication channel without influencing the control system. Adapters, gateways and edge devices provide the necessary connectivity on old and new plants. In the future, the Advanced Physical Layer will even enable fast two-wire Ethernet in hazardous areas.

It would be worthwhile to treasure the data from process analytics. This is because, in addition to a deeper understanding of the process and better process control, process analytics also enables knowledge to be preserved, as it provides relevant information about the process. Quality managers obtain a large database that they can use to initiate fundamental changes and minimize deviations in product quality. Evaluations of these data allow, among other things, the identification of "golden batches."

In addition, the numerous data available in the device on condition and operating history support condition-based maintenance and maintenance personnel in the event of damage. Digital services are already available today that make all field devices and their data accessible from anywhere. The applications (apps) help users, for example, to record and manage all the instruments in a plant, organize device-related documents, or monitor the device status and act correctly in the event of a malfunction.

Remote maintenance systems also allow PAT experts to support maintenance personnel in a plant without having to go onsite themselves. If a fault condition is detected or suspected, a more detailed condition assessment can be carried out, and repair measures can be prepared in a more targeted manner. During onsite maintenance, mobile devices are used with which maintenance personnel can access electronic documentation on site, maintain maintenance histories in the computerized maintenance-management system (CMMS) or initiate procurement processes electronically. ■

Edited by Gerald Ondrey

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PAT is IIoT Ready

Combining process analytical technology (PAT) and the cloud for next-level productivity

Martin Gadsby
Optimal Industrial Automation Ltd.

IN BRIEF

FUTURE CPI PRODUCTION IS PAT-DRIVEN

PAT AND SMART ARE INTERCONNECTED

NEXT-GENERATION PAT

ACT NOW FOR A COMPETITIVE EDGE

FINDING THE IDEAL PAT SYSTEM

Process analytical technology (PAT) enables manufacturing and processing companies to continuously enhance their competitiveness in an increasingly fast-paced and demanding market (see part 1, "Process Analytical Technology Advances," pp. 24–31). The latest advances in data technology — particularly cloud computing — can help create an advanced PAT framework and new opportunities for manufacturers. As a result, companies can improve flexibility, responsiveness, efficiency and quality across an entire enterprise.

PAT is among the key solutions that forward-looking businesses should implement when developing smart manufacturing strategies (Figure 1). It is a realtime, data-driven framework that aims to improve process efficiency, resilience and quality by controlling critical process parameters (CPPs) within a pre-defined design space to optimize a product's critical quality attributes (CQAs) in a timely manner. At the core of this setup is an in-depth, science-based understanding of how CPPs influence CQAs that allows businesses to implement quality-by-design (QbD) practices, where quality is built into products from the early design phases.

Future CPI production is PAT-driven

This knowledge supports the implementation of statistical process control and the creation of models for quality predictions. As a result, it is possible to make sure that all manufacturing activities are operating according to the most effective processing conditions at all times, enabling companies to consistently deliver high-quality products and reduce variability while optimizing a plant's operations.

In addition, by supporting realtime monitoring either in-, on-, or at-line, PAT allows chemical manufacturers to move away from offline laboratory analysis and adopt more comprehensive, as well as faster, process analytics. This transition results in a considerably improved process understanding and enhanced root-cause strategies, while also minimizing the downtime associated with quality control. For example, it is estimated that the downtime associated with quality control/assurance can be halved and the cost of quality (CoQ) can be reduced by 15% [*1*].

Furthermore, a PAT system can help ensure regulatory compliance as well as lay the groundwork for the implementation of lean-manufacturing and six-sigma strategies. By reducing off-specification materials via realtime quality-assurance practices, chemical processing facilities can substantially reduce waste and reworks, minimize raw material and energy utilization, as well as shorten production times. Consequently, it is possible to reduce time-to-market and support just-in-time manufacturing.

Live process control can also help to reduce overprocessing and achieve homogeneous product quality, for example, by obtaining a narrow particle-size distribution during granulation phases, further streamlining manufacturing activities [*2*].

Considerable savings in operational expenses (OPEX) are therefore achievable. Similarly, it is possible to optimize existing assets, reducing the need for significant new investments to increase capacity. For instance, biologics manufacturers that have adopted PAT-driven strategies have reported a threefold increase in titers (capacity) from their fed-batch units [*3*]. This shows that capital expenditure (CAPEX) can be optimized using the insight provided by PAT to support continuous improvement strategies.

FIGURE 1. An advanced PAT framework, such as this commercial system that utilizes cloud computing, can help to create new opportunities for manufacturers

PAT is also key to enabling the adoption of continuous processing strategies, which can further streamline production and processing operations, reducing running costs, cycle times, energy and resource utilization. In particular, a study examining the fractional cost differences between operating continuous flow and batch reactors in chemical manufacturing plants concluded that operating costs are between 15 and 40% lower when continuous processes are used [*4*]. More precisely, a fourth of costs for catalysts were required in hydrogenation stages while 35% could be saved in expenses associated with energy usage during nitration [*4*].

PAT & 'smart' are interconnected

To provide successful, data-driven insight into processing activities with PAT, a highly interconnected infrastructure needs to be created that can transfer, store, process, analyze and subsequently visualize the large volumes of information continuously generated. To implement an effective industrial internet of things (IIoT) system, manufacturers need to move away from conventional, centralized high-performance computing strategies that focus on supercomputers or clusters of collaborative computers. Instead, they should favor high-throughput computing, which relies on distributed data sharing and content delivery applications. As a result of this paradigm shift, it is necessary to develop suitable data fusion strategies that can facilitate the integration of readings from different instruments to create optimized quality predictions and a comprehensive process overview.

PAT can address these needs using the latest innovations in sensor and network technologies, big data analytics and data mining. In effect, it can support the creation of a highly interconnected, comprehensive and intelligent system that enables industry 4.0 applications. This ultimately facilitates next-level realtime process control and quality assurance.

While big-data technologies are extremely important, it is also essential to create a suitable infrastructure that can support them. One of the most promising enabling technologies is cloud computing, as it offers near unlimited space for storage and data processing power on demand, as well as decentralized data availability (Figure 2). Hence, it is a key tool for chemical manufacturers interested in setting up big-data-driven process intelligence strategies aimed at enhancing their operations and end-product quality.

FIGURE 2. The cloud can enable the creation of an enterprise-wide PAT system, which is able to acquire and integrate key knowledge from multiple manufacturing facilities, regardless of their geographical location

Next-generation PAT

The next generation of PAT should support data transfer to the cloud. The cloud allows companies to truly leverage the power of big data by providing a flexible stack of massive computing, storage and software services in a scalable manner and at a low cost. It offers this without the need to build the required physical high-capacity computing infrastructures that need substantial CAPEX and OPEX as well as increase the manufacturing footprint.

A practical example can be found in (Fourier-transform) near-infrared (NIR) process spectrometers, which are able to generate multiple spectra per second. The volume of data produced by a single analyzer, let alone a network containing multiple analyzers, can quickly exceed the gigabyte range. Therefore, existing on-premises servers and data centers in chemical plants may not have the ability to store and analyze such large datasets from multiple devices and analytical instruments.

While edge computing is generally better suited to support time-critical process control, the cloud is well-equipped to address the needs of advanced process control during predictive model-building phases. In particular, cloud computing can support the creation of an extremely advanced PAT knowledge-management system that can perform complex functions and computing algorithms, which require more computing power than can be possibly provided by edge-computing devices. Time-critical model execution can then be delegated to real-time control systems, such as programmable logic controllers (PLCs) and distributed control systems (DCSs), which are acting on quality-driven setpoint changes from the cloud-based PAT system. These will then work together to automatically adjust CPPs, thus optimizing quality. Consequently, a PAT solution that can pump data to the cloud can help chemical manufacturers to set up advanced, automated operations that increase production flexibility and responsiveness.

An additional benefit of utilizing a framework that supports cloud connectivity is that companies can set up an enterprise-wide PAT system, which is able to acquire and integrate key knowledge from multiple manufacturing facilities, regardless of their geographical location. By doing so, chemical manufacturers can gather larger volumes of data, creating ever more accurate and precise predictive models. Furthermore, they can standardize processes across multiple plants, creating shared best practices. Such a system can also support multi-site collaborations and coordination. Ultimately, chemical manufacturers can optimize all aspects of their operations while increasing consistency across different factories.

Optimal

FIGURE 3. A data driven PAT framework, such as the commercial system shown here, can help manufacturers to greatly improve flexibility, responsiveness and product quality

Moreover, cloud-computing solutions are fully scalable, supporting expansions and upgrades within chemical manufacturing plants, even for limited periods of time. This is particularly beneficial for chemical manufacturers during model validation, as they can scale-up data processing capabilities temporarily and downsize when these activities are not required.

Data transparency and availability are also enhanced by the cloud, with multi-user access and remote monitoring supported. Also, if equipped with instant reporting capabilities, a PAT solution that supports cloud computing can facilitate and streamline the creation of suitable documentation for quality auditing or similar purposes.

Finding the ideal PAT system

To get the most out of cloud computing for process control and quality assurance, companies need to choose a PAT knowledge-management platform that can effectively pump data to the cloud. This will either utilize either "push" or "pull" methods for data transfer. In the former, data are periodically sent by each monitored system to a central data lake located in the cloud. Whereas in a "pull" architecture, a central collector periodically requests metrics from each monitored system.

Each data-transfer method benefits different applications and the specific requirements of an enterprise. For example, if advanced cybersecurity is a top priority, a PAT data pump system based on "push" methods is likely to offer the best solution, as it can support controlled access. Setting up such a system is therefore extremely important for producers supplying highly regulated industries, such as the pharmaceutical sector. More precisely, a "push" cloud-data pump prevents a network opening to a secure good-manufacturing practice (GMP) area containing the PAT's comprehensive data. In either case, populating a cloud-data lake provides companies with the ability to expand their data-driven science using their best, established tools without accessing secure systems directly.

In addition, it can prove extremely beneficial for chemical processing and manufacturing facilities to adopt a PAT system that is able to transfer and store data in the cloud that complies with current good-manufacturing practices (cGMPs) and directives for food and pharmaceutical producers. In this case, companies need a PAT solution with cloud-data-pump capabilities that can meet regulations on electronic signatures and records (ERES), such as the European Union's GMP Annex 11 or the U.S. Food and Drug Administration's (FDA) 21 CFR part 11, or both. Examples of products that support data "push" to the cloud, while addressing governing standards of the pharmaceutical industry, are available.

Act now for a competitive edge

A PAT system can already offer a major advantage to chemical manufacturing facilities by interfacing with analyzers. The importance of PAT will continue to increase as companies need to create data-driven applications and highly interconnected infrastructures to realize smart manufacturing strategies. The opportunities and innovations offered by industry 4.0 technologies are also able to enhance the capabilities of PAT and increase the benefits of this framework (Figure 3).

In particular, a PAT framework that supports cloud computing for data analysis, storage and reporting can greatly improve flexibility, responsiveness and product quality while reducing waste, costs, energy and resource utilization. In order to fully reap the benefits of this technology, it is important for chemical manufacturers to identify a solution that can meet the needs of their enterprise and is secure, regulatory compliant and easy to access. By selecting the right system, chemical manufacturers can leverage a unique competitive advantage while future-proofing their operations. ■

Edited by Gerald Ondrey

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Modularization: Managing Project Delivery Risk in the Time of COVID

Taking a modular approach to capital projects offers a pathway for companies to be proactive, rather than reactive, as they manage project risk in the time of COVID and potential similar disruptions in the future

Mauricio Villegas and Chris Loftus
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IN BRIEF

COVID-19 RESPONSE

MODULAR CONSTRUCTION DEFINED

DELIVERY, INSTALLATION AND STARTUP

MODULARIZATION BENEFITS

PREPAREDNESS FOR PROJECT RISK

OLD PROBLEMS; MORE CHALLENGES

THE PATH FORWARD

It has been more than a year since the COVID-19 global pandemic took center stage, and the uncertainty engendered by it has impacted every person on the planet. The disruption of the pandemic precipitated a cascading series of changes observed across nearly every industry. It was no longer business as usual. Although the chemical process industries (CPI) are familiar with the cyclical nature of the markets into which they sell, for the first time, the CPI faced a paradox: how to continue to execute projects on time and on budget, while keeping contractors, employees and operators safe in the midst of a public health crisis. The need to address this issue applies not only to current projects in the time of COVID-19, but also to future projects, which may face unknown and unanticipated risks from forthcoming health crises, natural disasters or other widespread disruptions. This article provides information on how modularization can help manage project risks in the new environment in which CPI companies now find themselves.

FIGURE 1. The truckable process module shown here is being readied for transport to a project site

COVID-19 response

In a matter of weeks after COVID-19 was first identified, both plant owners and engineering, procurement and construction (EPC) firms alike were implementing stay-at-home orders and sending employees home to work virtually to ensure their safety and help slow the spread of disease. Even prior to the pandemic, many in the CPI were already familiar with virtual team environments, simply from having to manage project teams across various geographic regions to facilitate work sharing. So in some ways, companies were well positioned remotely and virtually executed design- and engineering-related work. Even as the percentage of remote workers rose and strained the information technology (IT) infrastructure, the CPI answered the call successfully.

However, neither "greenfield" nor "brownfield" projects can be physically constructed in a virtual environment. The same challenges brought on by the procedures designed to ensure that workers remained safe also began to materially impact construction projects, particularly those employing traditional stick-building construction strategies. Addressing these challenges directly impacted the CPI's collective ability to deliver projects safely. As a result, schedules and budgets started to slip.

FIGURE 2. Once delivered to a project site, truckable modules are set on pre-made foundations

Health and safety risks became the primary constraint on continuing project execution and field operations. Fairly abruptly, companies' focus shifted from reducing workplace hazards to managing workforce COVID-19 exposure and infection rates. There was a widespread feeling of community and social responsibility to prevent community spread of the virus. A number of health and safety preventative measures are now common practice, and many have become normalized, including social distancing, additional personal protective equipment (PPE), pre-work measurement of body temperatures and staggering lunch breaks and work shifts to reduce gatherings and exposure.

Incorporating these new policies and procedures impacts the engineering and planning components of project delivery in several ways, including the following:

- Construction challenges
- Completion date slippages
- Critical work activities extended
- Deferred startups and commissioning activities
- Extension of project schedule
- Flattening of expenditures across the project duration
- Lower levels of project productivity

In addition to the onsite challenges, few anticipated the extent to which global supply chains were disrupted in the wake of the pandemic. Supply chain disruptions, in turn, had cascading effects that led to the following:

- Schedules and project scopes requiring rework
- Shifting priority to projects that could deliver immediate return on investment (ROI)
- Shifts in the pipeline of planned projects
- Delayed final investment decisions
- Projects being revisited and re-evaluated
- Reductions in capital expense (CAPEX) budgets
- Delays in project approvals

In light of these new challenges, realization took shape that the advantages and benefits inherent to modular construction strategies could help mitigate many of the project-delivery risks that arose with COVID-19. While it is true that, even with modular construction approaches, physical projects cannot be accomplished virtually, it is also the case that modularization could help companies adapt to many of the supply-chain, project-scheduling and health-safety issues associated with the pandemic. In fact, modular construction has always provided some of these benefits.

Modular construction defined

Modular construction of process systems can be defined as complete process units that are prefabricated at an offsite, specialized, indoor, modular assembly shop to the maximum extent possible.

Truckable modular systems, as an example, are built in such a way that they can be transported across states and countries by trailer truck (Figure 1). The modules are supported by a structural steel frame, which serves not only as the support system for the equipment during shipment, but once installed, allows for a safe passageway via access platforms to operate.

In general, building systems under controlled indoor environments minimizes field construction labor by up to 90%, and mitigates the inherent risks associated with field construction.These legacy benefits of modular construction align well with addressing concerns surrounding project execution during COVID-19 or another similar disruption in the future.

Delivery, installation and startup

Given that many truckable modular-process-unit providers are experienced in the delivery of their modules to owners' sites — both domestic and globally — delivery is included in the overall scope of modular construction, in most cases. In preparation to receive modules onsite, the facility owner's onsite construction contractor will prepare the foundations where the modular systems will be set upon arrival. The foundations are prepared based on foundation load drawings provided soon after the purchase order for the modules is prepared (Figure 2).

Depending on the number of process modules comprising the overall project and the overall onsite project construction completion status, modules can either be received onsite all at once, by staggered shipment or received and set on temporary supports in the laydown yard. Typically, smaller projects comprised of one, two or just a few modules can be received and set in a single day. Larger projects comprised of a series of modular systems will have delivery staggered over the period of a few weeks.

Once the modules are in place and all interconnecting spools have been installed, the process units are connected to the outside battery limits (OSBL) utilities, feed piping and product pipelines. After the completion of a field-readiness checklist, a mock startup is performed using water. It is important to do a water startup prior to introducing chemicals into the process units to ensure all instrumentation and equipment is working properly. This reduces potential exposure to hazardous chemicals. Once the system has been validated using water and controls have been adjusted in the control room, the plant is ready for full commissioning and startup with the process chemicals. Depending on the size of the plant, typically one or two engineers, plus an operator, are required during startup. This allows for opera-

IMPACT OF COVID-19 DURING FABRICATION: AN AMMONIA RECOVERY SYSTEM CASE STUDY EXAMPLE

This case study concerns a modular construction project that had kicked-off six months prior to the quarantine mandate in the northeastern U.S.

The project involved an ammonia recovery system that included three truckable process modules and one stair tower (Figure 4). The project schedule was 49 weeks, including process development, detailed engineering, procurement, fabrication and shipping to the client's site. When COVID-19 hit, the project was at the beginning stages of the modular assembly phase: process design and detailed engineering was complete; structural steel nearing galvanizing; equipment and instruments were approaching readiness for shipment to the modular assembly shop; and the modular assembly contract was already awarded.

Supporting the project from home offices, rather than a company office setting, became the first challenge. During this time, most individuals had to continue their work activities from home. One of the first advantages of modular construction that came to light is that the construction staff did not change, and the relationship of the project manager with the selected assembly shop had been established for years prior to the pandemic. This would have been a very different situation for a stick-built project, where workforces are mobilized from different parts of the country.

FIGURE 5. The stripping column of the ammonia recovery unit is shown here

Using technology resources to connect with and manage resources, such as video conferencing, email, and phone calls, allowed for a smooth transition and efficient, effective communication.

A vendor responsible for delivering three vessels that would go into the modules confirmed that the vessels had been completed and were ready for the final hydrotest, as well as for the installation of the internals. However, when the inspector and engineer arrived, they were notified that one of the vessels was not yet complete. The inspector and engineer extended their trip long enough to see that vessel through hydrotest, but had to return before the internals in the third one could be installed, because COVID case numbers were quickly increasing at the time, and new protocols (including restaurant closures) were quickly going into place. Because of the fear of not being able to safely return to the vessel shop, the three vessels (along with the uninstalled packing for the third column) were sent to the assembly shop with plans to install the packing in the third one at the assembly shop, which had the full set of equipment needed to do this work under roof (Figure 5). To ensure the safety of the assembly shop employees as the virus case rate continued to increase, a detailed procedure was drawn up and the engineers worked remotely with the assembly shop using a video camera and sequential pictures to support this work.

FIGURE 4. The photo shows one of three truckable process modules for the ammonia-recovery unit discussed in the sidebox

Another important focus during the modular assembly phase was to keep the assembly shop employees healthy. Modular construction is performed with an assembly line approach, which requires low workforce density. The modules are built along a horizontal orientation, allowing for reduced personnel hazards and other risks. Social distancing was possible with this type of arrangement. This is in contrast to the situation at a stick-built facility, where workers perform activities simultaneously, often in close quarters in multiple areas around the construction site.

The assembly shop also added additional measures of its own to ensure the project would be successful. Weekly staff meetings were scheduled to set the tone to keep the facility open and the importance of collaboration with the employees to stay healthy. Discussions about the impact of decisions made outside of the assembly shop, not only by the employees themselves, but also by their families, became routine. An emphasis was placed on the importance of individual behaviors.

It was key to understand the new risks and efficiently communicate with the various teams during assembly. The decision to shift the schedule to push for inspections and walkthrough toward the tail end of the project was made. This helped reduce exposure with outside personnel during construction.

The client was able to visit the assembly shop once the modules were near completion and was extremely satisfied with the way the team had handled the challenges brought by the global pandemic.

Recognizing all the challenges in a timely matter while also looking for proactive solutions resulted in zero cases of illness and the seamless, continuous production.

While the modularization part of the project allowed many challenges to be overcome, the client still faced other challenges that could not be avoided. For example, significant delays in permitting resulted from the local permitting office had closed due to the health concerns and with reduced staff returning to work, the timeframes were significantly extended to get approval of the permits.

This ammonia recovery system was completed on schedule, but the client shared that unfortunately, as a result of COVID-related delays, the foundation work had not yet been completed.

At time of modular readiness to ship, client requested that the modules be stored off-site at a laydown yard until all on-site work could resume and be finalized. Subsequently, hydraulic lift trucks were used for the modular transit and there was no need for cranes for unloading. ❑

tor training, while also ensuring that the unit reaches steady-state operation in a smooth matter.

With approximately 90% of the overall construction activities transferred to the modular assembly contractor, onsite installation, startup and commissioning activities are typically shortened from months to weeks, and onsite construction personnel required to support project scope is drastically reduced. Furthermore, associated costs related to onsite cranes and other rental equipment can be minimized, because they can be planned for use on site only when modules are being received and installed upon their foundations.

Modularization benefits

The benefits of modular construction that were recognized even before the global pandemic have only become amplified in the years 2020–2021. These benefits can be divided into three main categories: completion; contractual and commercial; and project risk mitigation. Included here is a list of benefits, some general and others more specific to COVID.

Completion. The benefits of modular in the area of construction completion include the following:

- *Increased productivity, quality, and safety at the indoor modular assembly shop.* The step-by-step, assembly-line method of construction allows for predictable procedures, reduces the risk of injury to personnel and improves overall product quality
- *Minimized interruption to the owner's site operation* resulting from offsite fabrication and assembly, along with short times onsite for installation, startup and commissioning activities
- *Significant schedule improvements* over traditional stick-built projects
- *Better labor availability.* Assembly shops have a more stable workforce and do not experience the typical personnel turnaround that is seen with pulling stick-built construction crews together for each project
- *Continued off-site fabrication* during site-permitting activities
- *Smaller workforce* equates to less non-productive time spent performing the newly necessary pre-work health screening
- *Controlled work environment* contributes to higher productivity in inclement weather
- *The ability to shift fabrication to multiple assembly shops* in locations with low COVID-incidence rates. Modular construction allows you to change the fabrication site to areas with lower case rates, something that could not be accomplished with a stick-built approach
- *Mitigated labor availability disruption* by minimizing workforce exposure and infection in these controlled environments
- *Maintained productivity* during a pandemic mitigates schedule extension

The owner of the plant is able to see significant improvement in overall project execution when activities are performed in a parallel fashion, versus when performed sequentially. Modularization allows the end-user to focus on activities such as acquiring necessary permit approvals from local municipalities, without causing delay in the design and construction of the process units, normally ongoing in the modular shops already. This is one example of how schedules are shortened, with the modules ready for shipment within 10 months of kicking off the project. This is, and has always been, very difficult to accomplish with stick-built construction.

Contractual and commercial benefits. Modular construction has always delivered contractual benefits and risk mitigation. This has not changed during the pandemic, but the approach is being looked at with fresh eyes. A third-party modular systems provider will assume fabrication and delivery risk of the completed modular system, taking on much of the project delivery risk. This transfers some risk from the facility owner to the contractor. There is also a definitive estimate, and fixed price scenarios, which can provide overall cost savings.

FIGURE 3. Modular process equipment can be put together in an assembly-line fashion, which allows lower workforce density

Additionally, maintaining contract performance requirements is paramount for the successful execution of a project. By minimizing workforce exposure, infection rates and supply chain disruptions, plus maintaining labor availability, modular approaches enable a smooth process for execution and fabrication.

On the contract side, there is a risk reduction on force majeure, suspension of work, and stop work order. On the commercial side, the risk of increased project costs related to extended performance and legal costs and contract penalties are reduced.

Project risk mitigation. When considering a modular execution model over stick-built construction, various project delivery risks can be mitigated through modularization. This has always been the case, but when viewed through a pandemic lens, it highlights certain aspects even more clearly.

While a typical stick-built construction site workforce could require hundreds or thousands of individual workers, an indoor modular assembly shop may average under 100 workers in one location. This allows for the following:

- Assembly line fabrication methodology that equates to smaller workforce density (Figure 3)
- Overall smaller shop workforce population
- Smaller field size population
- Controlled environment, which offers greater PPE comfort and higher compliance
- Shorter exposure duration
- Local and consistent workforce that minimizes potential community spread

Preparedness for project risk

Preparation is key to helping minimize project risks as the industry continues to adapt to this ever-changing landscape. The pandemic highlighted some weaknesses in the marketplace that can now be addressed in cases where similar circumstances develop in the future. For example, there are some steps that owners can take early on during the planning of a project that allows for a more proactive execution.

These include the following items:

- Performing risk assessments on future projects to include likelihood of an epidemic or pandemic
- Understanding local permitting timeframes
- Close collaboration between the engineering firm and module supplier to identify bottlenecks early in the planning phase of the project
- Identifying site workforce availability to minimize bringing workers from outside the local geographic area
- Soil testing and subsequent foundation preparation and construction
- Identifying potential lay-down areas if required
- Securing supply chain early in the project to minimize impact of a heated market premium

Old problems; more challenges

CPI companies have overcome many obstacles in the last few decades, such as the financial crisis of 2008, and the global recession of 2014. Many could say that the problems faced during the pandemic were simply old problems in a new global landscape, but the numbers tell a different story. This single event is still causing unique challenges in the industry. According to Industrial Information Resources (Sugar Land, Tex.; www.industrialinfo.com), the pandemic has directly impacted more than 7,000 projects globally worth $556 billion. Specific actions were announced throughout the industry. For example, Fluor Corp., one of the largest EPC players in the industry, announced its exit from competitive EPC lump-sum bidding in 2020 on its full-year 2019 press release. Key reasons driving this decision were the increased project risk, the transactional marketplace, and ultimately, the market uncertainty driven by the COVID-19 pandemic.

And although many of the challenges are common in the industry, such as extension of project schedules, lower levels of project productivity, CAPEX budget cuts and so on, the reality is that these current challenges "feel" different. It is the first time in over 100 years that the industry is fighting with a new and possibly fatal pathogen on such a widespread basis. EPC activities will continue to be impacted, but companies will continue to adjust. Perhaps the best lesson is better preparation.

The positive news is that owners can take steps early on during the planning of a project that allows for a more proactive execution. Preparation is key to help minimize project risks as the industry continues to adapt to this ever-changing landscape. The pandemic highlighted some weaknesses in the marketplace that can now be addressed in case similar circumstances develop in the future.

As mentioned earlier, there are some key steps that owners can take early on during the planning phase of a project. These steps range from performing risk assessments on future projects to include the likelihood of an epidemic or pandemic, to securing the supply chain early to minimize the impact of a heated market premium. Also, understanding local permitting timeframes highlight the importance of strong contractor relationships. Taken together, these steps allow for a more proactive and risk-mitigated project execution.

The path forward

The reality is that nobody can predict when the pandemic will be over, if it will be the last one our industry will face or what the new steady state will be five years or even ten years from now. What is clear is that the industry needs a project-execution model that enables projects to continue to be delivered successfully and safely in challenging environments. Modular construction can help level the playing field due to its adaptive nature.

Modular assembly shops also continue to mitigate the impact of the pandemic. Executing a project in this fashion allows for continuous operation at the owner's facility with minimum interruption, which is possible while maintaining the proper health and safety measures.

Ultimately, modularization can serve as a potential risk-mitigation approach as the industry adapts to what will be the new normal. While it would be simplistic to say that modularization is the silver bullet to the COVID-19 pandemic's ongoing challenges to the delivery of projects, modular construction, together with other project-risk-mitigation measures, can and has played a significant role in enabling projects to continue safely and effectively. It should be considered as a viable alternative, both in the current situation and into the future.

The pandemic highlighted weaknesses in the marketplace that can now be addressed in anticipation of similar circumstances in the future, which in light of history and public health research, will very likely occur. ■

Edited by Scott Jenkins

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Changing Fluids in a High-Temperature Heat Transfer Fluid System

Switching from one fluid to another in a heat transfer system requires an engineering evaluation. Here is what to include

Gerald E. Guffey II
Eastman Chemical Company

In well-designed and well-maintained heat transfer systems, heat transfer fluids generally last for a long time and function as intended. However, there are situations in which it is necessary to change heat transfer fluids. When a switch in fluids is required, facilities in the chemical process industries (CPI) should pay careful attention to a number of important considerations surrounding the properties of the old and new fluids, as well as the design of the heat transfer system. This article provides information about conducting an engineering evaluation to determine how the fluid change will affect safety, environmental concerns, system maintenance and process performance.

Heat transfer system operation

Steam is often used for process heating. Primarily, steam transfers heat when it condenses. To transfer heat at high temperature, the steam pressure must be very high. For example, 600-psig steam condenses at approximately 490°F, but many processes require heating to higher temperatures than that. For these applications, a heat transfer fluid can be used. Heat transfer fluids are sometimes referred to as thermal fluids or hot oils.

Heat transfer fluids have a much lower vapor pressure than water, so they require a much lower operating pressure at a given temperature. Also, a heat transfer fluid system can be designed to provide both heating and cooling to a process, if required.

Some systems are designed to use heat transfer fluid in the vapor phase, but most systems use heat transfer fluid in the liquid phase. A typical liquid-phase heat transfer fluid system, as shown in Figure 1, includes a heater, a pump to circulate fluid through the heater to the process, an expansion tank to accommodate thermal expansion of the fluid, and one or more process heat exchangers. Subloop pumps may be used to circulate fluid through process heat exchangers. Sometimes subloops are operated at a lower temperature than the main circulating loop, and fluid from the main loop is only added as needed to maintain the desired operating temperature. System volume can vary from a few gallons for a pilot-scale system to over 100,000 gallons for a large-system with multiple heaters.

Heat transfer fluids degrade over time when operated at high temperature. Thermal degradation products include low-boiling components, high-boiling components and sludges. In a well-designed and well-maintained system, the fluid should last for many years. The condition of the fluid should be routinely monitored to assess when fluid maintenance is needed.

Considering a fluid change

Plant owners with a heat transfer fluid system may decide to switch fluids for several reasons, including the ones listed here:

Rapid performance degradation. The current fluid performance has degraded too quickly at the current operating temperature. There may be fouling of heat exchangers by high-boiling solids in the degraded

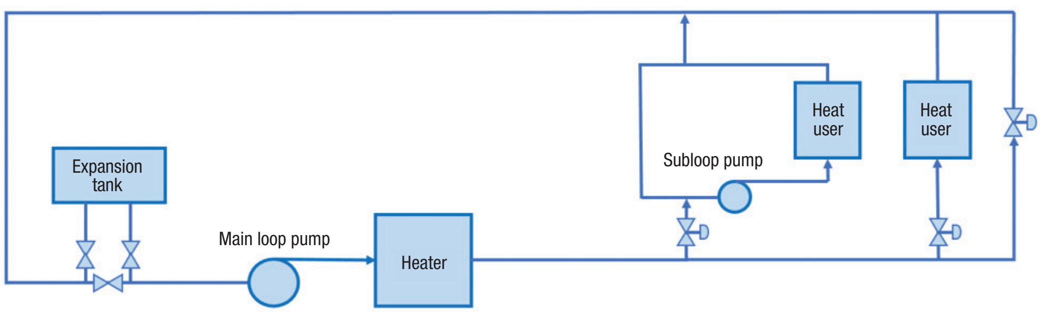

FIGURE 1. This process diagram shows a typical liquid-phase heat transfer fluid system

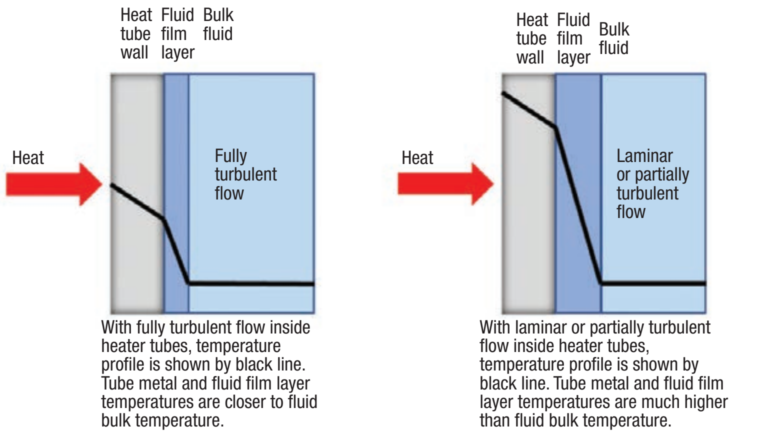

FIGURE 2. The black line represents the heat transfer fluid's temperature profile inside the heater tubes

fluid, which can reduce heat transfer to the process. A significant level of low-boiling components in the degraded fluid may be accumulating in the heat exchangers, which can reduce heat transfer to the process. Similarly, accumulation in pumps can reduce pump output. These problems can limit production rate.

Need higher temperature. The owner may be planning to increase the system operating temperature to increase heat transfer to the process, and the current fluid will degrade too quickly at the higher temperature.

System-fluid mismatch. The owner has discovered a mismatch between the system design and the current fluid. As an example, the author has seen a system where the selected fluid's vapor pressure at operating temperature was higher than the pressure rating of the expansion tank and some other components, so fluid was continuously being vented out of the system.

Cost considerations. The owner may be trying to reduce cost. However, the ongoing cost to add fluid to the system must be considered, as well as the initial fill cost. A fluid that is more resistant to thermal degradation will have lower ongoing cost for makeup fluid, and fewer issues with fluid degradation products.

Supplier technical support. The owner may need a more extensive level of technical support from the fluid supplier. The owner can benefit from an experienced fluid supplier with deep knowledge of fluid chemistry who can provide detailed information about why the fluid condition is changing and make practical recommendations about what actions are needed. In the event of fluid contamination, an experienced supplier can evaluate the impact and help the owner determine what actions to take.

Comparing fluids

The most common high-temperature heat transfer fluids are synthetic organic fluids, mineral oils and silicone-based fluids. Most heat transfer fluids have unique chemistries, so their physical properties are different. Because fluids have different physical properties, it is always appropriate to do an engineering evaluation to determine how the fluid change will affect safety requirements, environmental requirements, operation and maintenance of the system. The engineering evaluation should include all of the factors described below.

Fluid temperature ratings. Heat transfer fluids have maximum bulk-temperature and maximum film-temperature ratings that vary by chemistry and are determined by the fluid supplier. Bulk temperature is the temperature that the majority of the fluid experiences. Film temperature is the temperature experienced by the film layer in contact with the heater tubes or heating element as heat is transferred into the fluid. Film temperatures are higher than bulk temperatures, so the thermal degradation rate experienced by the fluid's film layer is higher.

The volume of the film layer is small compared to total system volume. For systems with a well-designed heater operating at or below its design capacity, the amount of thermal degradation experienced by the film layer will be a small portion of the thermal degradation of the total system.

The heater should be designed for fully turbulent flow inside the tubes or across the heating element. This increases the heat transfer coefficient and decreases fluid film temperature and film thickness. A more conservatively designed heater will result in a smaller difference between the fluid film temperature and the bulk temperature, as illustrated in Figure 2.

There is no single, universal approach to determine fluid temperature ratings, so some suppliers may be more conservative with their ratings than others. Each supplier can explain how its fluid temperature ratings were determined. Thermal stability (the resistance to permanent changes in properties caused solely by heat) must be considered in determining fluid temperature ratings, since it strongly influences the life of the fluid. Thermal stability of fluids can be measured using ASTM test method D6743, the Standard Test Method for Thermal Stability of Organic Heat Transfer Fluids, which quantifies the amount of thermal degradation that the fluid experiences at a given temperature and time period. At its maximum bulk-temperature rating and maximum film-temperature rating, a fluid should have a thermal degradation rate that is sufficiently low that the fluid will last for many years.

In general, the selected fluid should have a bulk-temperature rating equal to or higher than the highest operating temperature of the system. Also, the fluid's film temperature rating should be equal to or higher than the highest film temperature that will occur in the heater. Film temperature is a function of the heater heat flux (heat transferred per unit area), as well as the fluid properties (which affect the heat transfer coefficient of the fluid). Film temperature is directly proportional to heat flux. Given the same fluid flowrate through the heater, an increase in heat flux (by increasing the firing rate of the heater) will result in an increase in film temperature. Film temperature is inversely proportional to the heat-transfer co-

efficient of the fluid film. Given the same flowrate through the heater and same firing rate, a new fluid with higher heat-transfer-film coefficient than the old fluid will experience a lower film temperature.

Fluid heat transfer properties. The effectiveness with which heat is transferred from the heat transfer fluid to the process is expressed by overall heat transfer coefficient. Equation (1) describes the heat transfer through a wall.

$$U = 1/h_P + L/k + 1/h_{HTF} \quad \textbf{(1)}$$

Where:

U is the overall heat transfer coefficient

h_P is the process-fluid-film heat transfer coefficient

L is the thickness of wall

k is the thermal conductivity of wall material

h_{HTF} is the heat transfer coefficient for the fluid film

The properties of the process fluid and heat transfer fluid influence the overall heat transfer coefficient. In some situations, the process side may dominate the overall heat transfer coefficient. In other situations, the heat transfer fluid side may dominate the overall heat transfer coefficient — in these instances, it is important to evaluate how changing the heat transfer fluid affects overall heat transfer coefficient.

The Sieder-Tate equation (Equation (2)) can be used to calculate the fluid-film heat transfer coefficient using fluid properties.

$$hD/k = 0.022\ (DG/u)^{0.8}\ (c_p u/k)^{0.4}\ (u/u_w)^{0.16} \quad \textbf{(2)}$$

Where:

h is the fluid-film heat transfer coefficient

D is the inside diameter of pipe

G is the mass velocity

k is the thermal conductivity at fluid bulk temperature

p is the density at fluid bulk temperature

c_p is the specific heat at fluid bulk temperature

u is the absolute viscosity at fluid bulk temperature

u_w is the absolute viscosity at fluid film temperature

The equation can be solved for the fluid-film heat transfer coefficient h:

$$h = 0.022\ (k/D)\ (DG/u)^{0.8}\ (c_p u/k)^{0.4}\ (u/u_w)^{0.16}$$

The terms can be regrouped in this manner, assuming that $(u/u_w)^{0.16}$ is equal to 1:

$$h = 0.022\ (D)^{-0.2}\ (G)^{0.8}\ (p)^{0.8}\ (c_p)^{0.4}\ (k)^{0.6}\ (u)^{-0.4}$$

Therefore, the ratio of fluid-film heat transfer coefficients for two heat transfer fluids is proportional to the ratio of their mass velocities, densities, specific heats, thermal conductivities and absolute viscosities raised to the appropriate exponent.

For heat exchangers where the heat-transfer-fluid side significantly influences the overall heat transfer coefficient, heat transfer to the process will be reduced if the new fluid has a lower heat transfer film coefficient than the existing fluid.

Fluid thermal expansion. Heat transfer fluids have a high coefficient of thermal expansion. Therefore, expansion tanks must have sufficient capacity to safely absorb the volume increase that the fluid experiences as it changes from the lowest temperature, when the system is down, to the highest operating temperature. It is good engineering practice to size the expansion tank to accommodate two times the volume change due to thermal expansion. Some systems utilize a smaller expansion tank located at the highest elevation of the system along with a larger overflow tank located at ground level. The combined capacity of these two tanks needs to be large enough to accommodate the thermal expansion of the fluid.

The amount of thermal expansion should be calculated for both the current fluid and for the new fluid. If the amount of thermal expansion for the new fluid is more than the amount for the old fluid, then expansion tank capacity must be checked to make sure that it is sufficiently large.

To minimize oxidation of the heat transfer fluid due to contact with air, the expansion tank should have an inert gas blanket. Oxidation will shorten the life of the fluid.

Fluid vapor pressure. A liquid heat transfer fluid system must operate at a pressure higher than the vapor pressure of the fluid at the operating temperature. Otherwise, some of the fluid will flash to vapor. The presence of vapor will cause pump problems and inhibit heat transfer. Low-pressure points in the system include the suction of the main loop circulating pumps, as well as the areas downstream of control valves that regulate flow from the main loop into subloops.

The expansion tank is typically connected to the return header just upstream of the circulating pumps for the main loop. The pressure of the inert gas blanket on the expansion tank can be set high enough to keep the system operating pressure above the fluid vapor pressure.

If the vapor pressure of the new fluid is higher than the vapor pressure of the old fluid, then the design pressure of system components must be checked to verify that all components can handle the higher operating pressure. In all cases, the sizing and setpoints of relief valves must be checked to determine if they are adequate for the new fluid.

Pump capacity and net positive suction head. If the new fluid has higher density than the old fluid at the operating temperature, then it will require more energy to pump it. The pump supplier should be consulted to verify that the existing pumps and drives will perform adequately with the new fluid. In some cases, a larger drive may be required.

The pressure of the inert gas blanket in the expansion tank should also be set high enough to provide adequate net positive suction head for the main loop circulating pumps. Net positive suction head required (NPSHR) versus pump flowrate is typically shown on the pump performance curve.

Net positive suction head available (NPSHA) can be calculated using this formula: NPSHA = expansion tank pressure – vapor pressure of the fluid at the operating temperature + static head between the expansion tank level and the centerline of the pump – pump suction piping losses.

NPSHA must be higher than NPSHR, or cavitation will occur and cause damage to the pump.

Pumpability. At low ambient temperature, the viscosity of any heat

transfer fluid increases, so it is more difficult to pump. If the new fluid has higher viscosity at low ambient temperature than the old fluid, then pumping it at low temperature will be more challenging. Heat tracing can be installed on pump suction piping to help warm the fluid. Also, pumps can be started with the discharge valve partially closed to prevent overloading the pump motor.

Some heat-transfer fluids solidify at ambient temperature. For these systems, heat tracing is needed to prevent solidification of the fluid inside transfer lines when flow is stagnant.

Fluid safety properties. Several properties can characterize the flammability hazard of a heat transfer fluid. Data on flashpoint, fire point and autoignition temperature are typically published by the heat transfer fluid supplier.

It is common for a heat transfer fluid system to have an operating temperature higher than the fluid flashpoint. The flashpoint is the lowest temperature at which an ignition source causes the vapors of the test sample to ignite under the specified test conditions. Examples of flashpoint laboratory tests are ASTM D92, which uses the Cleveland open-cup test apparatus, and ASTM D93, which uses the Pensky-Martens closed-cup testing apparatus.

Since flashpoint values are a function of the test apparatus design and test procedure, open-cup values should not be compared to closed-cup values. ASTM D92 also measures fire point, which is the lowest temperature at which the application of an ignition source causes the vapors of the test specimen to ignite and sustain burning for a minimum of five seconds under specified test conditions.

The operating temperature of the heat transfer fluid system should always be below the fluid autoignition temperature. Autoignition temperature is the minimum temperature at which autoignition occurs under the specified test conditions. ASTM E659 and DIN 51794 are test methods that measure the autoignition temperature of a fluid. The autoignition temperature of the new fluid should be higher than the highest operating temperature of the system.

Fluid initial boiling point. Heat transfer fluid systems should be designed to be leak-tight. It is good practice to avoid threaded piping connections and to minimize the number of flanges used. If a heat transfer fluid is heated to a temperature above its initial boiling point at atmospheric pressure, then accidentally leaked fluid will form some vapor and a mist cloud could result. If the new fluid will be heated to a temperature above its initial boiling point at atmospheric pressure, then plans for dealing with an accidental leak should be developed.

Environmental considerations. Used heat transfer fluids must be disposed of in accordance with local regulations. In the U.S., used heat transfer fluids are regulated by the Environmental Protection Agency (EPA; www.epa.gov) in 40 CFR part 279: Standards for the Management of Used Oil, which requires spill containment, a spill response plan and training. If leaked, some fluids have a spill reporting requirement. The heat transfer fluid Safety Data Sheet (SDS) should include information on accidental release measures, handling, personnel exposure and toxicity. The SDS for the fluid should be reviewed to ensure that adequate plans for containment, response, training and reporting are in place.

Implementing a fluid change

After the engineering evaluation has been completed, a plan for removing the old fluid, flushing the system, and filling with new fluid should be developed. A knowledgeable heat transfer fluid supplier will be able to help the owner develop this plan.

The old heat transfer fluid should be drained completely from the system through drain valves at low points in the system. Pressurized nitrogen may be used to help push fluid to the low points. If drains are not already in place at the low points, they will need to be installed.

After the system has been drained, the system can be filled with flushing fluid, which acts as a solvent to help remove thicker deposits of old fluid that may not have completely drained from the system. The flushing fluid should be compatible with all system components. The flushing fluid is typically heated and circulated throughout the system to remove deposits.

Chemical cleaning can be considered as an alternative to the flushing fluid. However, chemical cleaning is typically more expensive, and multiple flushes required during the cleaning process will generate more waste that must be disposed of.

After the flushing fluid has been drained, the system can be filled with the new fluid. If the system does not already have a side-stream filter installed, consider installing one to remove solids during operation of the system. Startup of the system with new fluid should include holding at about 220°F for several hours while circulating through the expansion tank to allow venting of moisture from the system. A blanket gas purge during the venting process can help greatly.

It is valuable to have a monitoring program to track the condition of the heat transfer fluid. Tracking key fluid parameters with trend analysis can detect changes in fluid condition before they become a problem. A monitoring program allows the fluid supplier to provide timely, practical recommendations for comprehensive maintenance for the heat transfer fluid system, so the owner can plan ahead to minimize the potential for an issue that might cause production downtime. ■

Edited by Scott Jenkins

Disclaimer

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2019 2020 2021

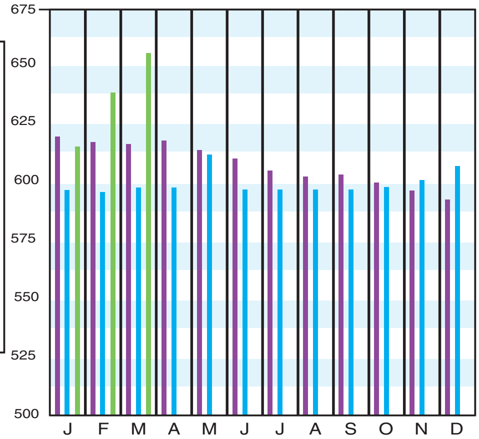
Download the CEPCI two weeks sooner at www.chemengonline.com/pci

CHEMICAL ENGINEERING PLANT COST INDEX (CEPCI)

(1957–59 = 100)	Mar. '21 Prelim.	Feb. '21 Final	Mar. '20 Final
CE Index	655.9	637.8	598.3
Equipment	808.5	782.8	726.2
Heat exchangers & tanks	698.4	675.3	621.4
Process machinery	792.5	771.1	724.7
Pipe, valves & fittings	1094.3	1052.6	954.7
Process instruments	474.6	450.7	416.8
Pumps & compressors	1111.9	1111.5	1085.2
Electrical equipment	586.3	575.4	562.3
Structural supports & misc.	877.3	847.0	778.5
Construction labor	333.8	333.6	335.7
Buildings	678.7	653.4	595.2
Engineering & supervision	310.2	310.8	313.4

Starting in April 2007, several data series for labor and compressors were converted to accommodate series IDs discontinued by the U.S. Bureau of Labor Statistics (BLS). Starting in March 2018, the data series for chemical industry special machinery was replaced because the series was discontinued by BLS (see *Chem. Eng.*, April 2018, p. 76–77.)

Annual Index:
2013 = 567.3
2014 = 576.1
2015 = 556.8
2016 = 541.7
2017 = 567.5
2018 = 603.1
2019 = 607.5
2020 = 596.2

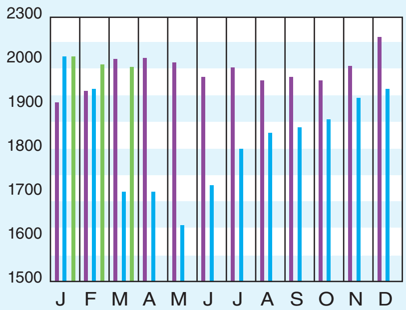


CURRENT BUSINESS INDICATORS

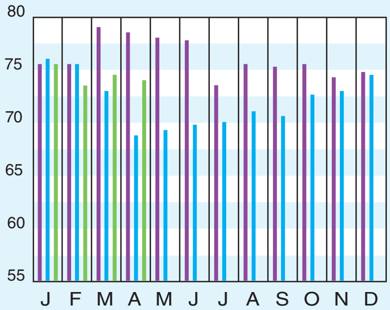
	LATEST	PREVIOUS		YEAR AGO
CPI output index (2012 = 100)	Apr. '21 = 99.4	Mar. '21 = 100.5	Feb. '21 = 100.5	Apr. '20 = 88.8
CPI value of output, $ billions	Mar. '21 = 1,827.7	Feb. '21 = 1,761.8	Jan. '21 = 1,761.8	Mar. '20 = 1,627.1
CPI operating rate, %	Apr. '21 = 74.3	Mar. '21 = 75.1	Feb. '21 = 75.1	Apr. '20 = 66.3
Producer prices, industrial chemicals (1982 = 100)	Apr. '21 = 296.1	Mar. '21 = 240.0	Feb. '21 = 240.0	Apr. '20 = 211.0
Industrial Production in Manufacturing (2012 =100)*	Apr. '21 = 103.2	Mar. '21 = 102.6	Feb. '21 = 102.6	Apr. '20 = 83.9
Hourly earnings index, chemical & allied products (1992 = 100)	Apr. '21 = 195.0	Mar. '21 = 194.3	Feb. '21 = 194.3	Apr. '20 = 193.6
Productivity index, chemicals & allied products (1992 = 100)	Apr. '21 = 101.2	Mar. '21 = 104.3	Feb. '21 = 104.3	Apr. '20 = 98.7

CPI OUTPUT INDEX (2000 = 100)†

CPI OUTPUT VALUE ($ BILLIONS)



CPI OPERATING RATE (%)



*Due to discontinuance, the Index of Industrial Activity has been replaced by the Industrial Production in Manufacturing index from the U.S. Federal Reserve Board.
†For the current month's CPI output index values, the base year was changed from 2000 to 2012
Current business indicators provided by Global Insight, Inc., Lexington, Mass.

CURRENT TRENDS

The preliminary value for the *CE* Plant Cost Index (CEPCI; top) for March 2021 (most recent available) indicates another large monthly rise, the sixth consecutive monthly increase. Similar to the story in February, the large uptick in March is linked largely to significant increases in producer prices for steel products, including carbon-steel sheets, plates and bars. These increases resulted in higher values for the both the Equipment and Buildings subindices. The Construction Labor rose slightly, while the Engineering & Supervision subindex fell by a small amount in March. The current CEPCI value now sits at 9.6% higher than the corresponding value from March 2020. The Current Business Indicators (middle) for April show a dip in CPI Output Index.